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CFD Investigation of Melt Spreading in the PULiMS-E10 Experiment

TESI DI LAUREA MAGISTRALE IN
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Abstract

The analysis of severe accidents in light water reactors requires a detailed understanding of the interaction between molten core material and coolant. In this context, underwater melt spreading plays a key role in determining the final debris bed geometry. The present thesis investigates the PULiMS-E10 experiment, performed at KTH, through a three-dimensional computational fluid dynamics (CFD) simulation developed in Simcenter STAR-CCM+.

The numerical model aims to reproduce the main hydrodynamic features of the experiment, with particular focus on melt release, underwater propagation, spreading over the bottom plate and accumulation. The water–melt system is described using a transient 3D Volume of Fluid approach. Since solving a single mixture energy equation led to an undesired cooling of the melt during the falling stage, the thermal field is instead described by two transport equations for the phase temperatures, one for the melt and one for the water, while the vapour phase is neglected. A simplified melt–water heat exchange is activated only below a prescribed depth in the pool, to reproduce, in an approximate way, the insulating effect of film boiling during the melt fall.

The progressive increase in melt viscosity due to cooling and partial solidification is represented through the Ramacciotti model, in which the apparent viscosity depends exponentially on an equivalent solid fraction obtained from the melt temperature. The numerical results are post-processed in terms of melt front propagation and are compared with the available experimental data from the PULiMS-E10 test.

The work provides an assessment of the capability and limitations of a simplified CFD approach for underwater melt spreading simulations. Although the model does not directly resolve boiling, fragmentation, crust formation, or full thermal solidification, it offers a computationally efficient framework for analysing the dominant spreading dynamics and the influence of cooling-induced viscosity increase on the final melt distribution.

Keywords: PULiMS-E10, underwater melt spreading, CFD, STAR-CCM+, Volume of Fluid, two-temperature model, Ramacciotti model.

Abstract in lingua italiana

L'analisi dei gravi incidenti nei reattori ad acqua leggera richiede una comprensione dettagliata dell'interazione tra il materiale fuso del nocciolo (melt) e il refrigerante. In questo contesto, il propagarsi del melt in acqua svolge un ruolo fondamentale nel determinare la geometria finale del letto di detriti. La presente tesi analizza l'esperimento PULiMS-E10, condotto presso il KTH, attraverso una simulazione tridimensionale di fluidodinamica computazionale (CFD) sviluppata in Simcenter STAR-CCM+.

Il modello numerico riproduce le principali caratteristiche idrodinamiche dell'esperimento, con particolare attenzione al rilascio del melt, alla propagazione sott'acqua, alla dispersione sulla piastra di fondo e all'accumulo del materiale. Il sistema acqua-melt è descritto mediante un approccio VOF 3D e transitorio. Poiché la soluzione di un'unica equazione dell'energia per la miscela portava a un raffreddamento indesiderato del melt durante la fase di caduta, il campo termico è invece descritto da due equazioni di trasporto per le temperature delle due fasi, una per il melt e una per l'acqua, trascurando la fase vapore. Uno scambio termico semplificato tra melt e acqua è attivato solo al di sotto di una profondità prestabilita, così da riprodurre in modo approssimato l'effetto isolante dell'ebollizione a film durante la caduta del melt.

L'aumento progressivo della viscosità dovuto al raffreddamento e alla parziale solidificazione è rappresentato attraverso il modello di Ramacciotti, nel quale la viscosità apparente dipende esponenzialmente da una frazione solida equivalente ottenuta dalla temperatura del melt. I risultati numerici sono analizzati in termini di propagazione del fronte e confrontati con i dati sperimentali del test PULiMS-E10.

Sebbene il modello non risolva direttamente ebollizione, frammentazione, formazione della crosta o solidificazione termica completa, esso offre una soluzione computazionalmente efficiente per analizzare la dinamica dominante della propagazione e l'influenza dell'aumento di viscosità sulla distribuzione finale del melt.

Parole chiave: PULiMS-E10, propagazione del melt in acqua, CFD, STAR-CCM+, Volume of Fluid, modello a due temperature, modello di Ramacciotti.

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1 | Introduction

1.1. Background and motivation

Nuclear energy is an important component of the global electricity mix, providing a low-carbon source of baseload power in several countries. According to the International Energy Agency (IEA), nuclear power accounts for approximately 9% of global electricity generation, with more than 410 reactors operating in over 30 countries [8]. Its role is even more significant in the European Union, where nuclear is the single largest low-carbon source of electricity and accounts for about a quarter of the electricity generated [6]. Together with its role in electricity production, nuclear technology requires extremely high safety standards, especially with regard to the prevention and mitigation of severe accidents.

A severe accident in a Light Water Reactor (LWR) may lead to core degradation and, in the most critical scenarios, to the formation of molten core material. If the reactor pressure vessel fails, this material can be discharged into the reactor cavity, where it may interact with coolant water and structural materials. The ex-vessel phase of the accident involves several coupled phenomena, including melt ejection, melt-coolant interaction, fragmentation, debris bed formation, melt spreading, and possible molten core-concrete interaction (MCCI) [20]. Figure 1.1 schematically illustrates the main ex-vessel phenomena that may occur following reactor pressure vessel failure.

The distribution of the molten material after vessel failure is a key aspect of accident progression. If the melt spreads over a large area, the resulting layer is generally thinner and can be more effectively cooled by the surrounding water. Conversely, if the material accumulates locally, a thick debris bed or melt pool may form, reducing heat removal and increasing the risk of long-term interaction with the cavity floor. For this reason, predicting the spreading behaviour of molten material is directly connected to the assessment of ex-vessel cooling strategies [10].

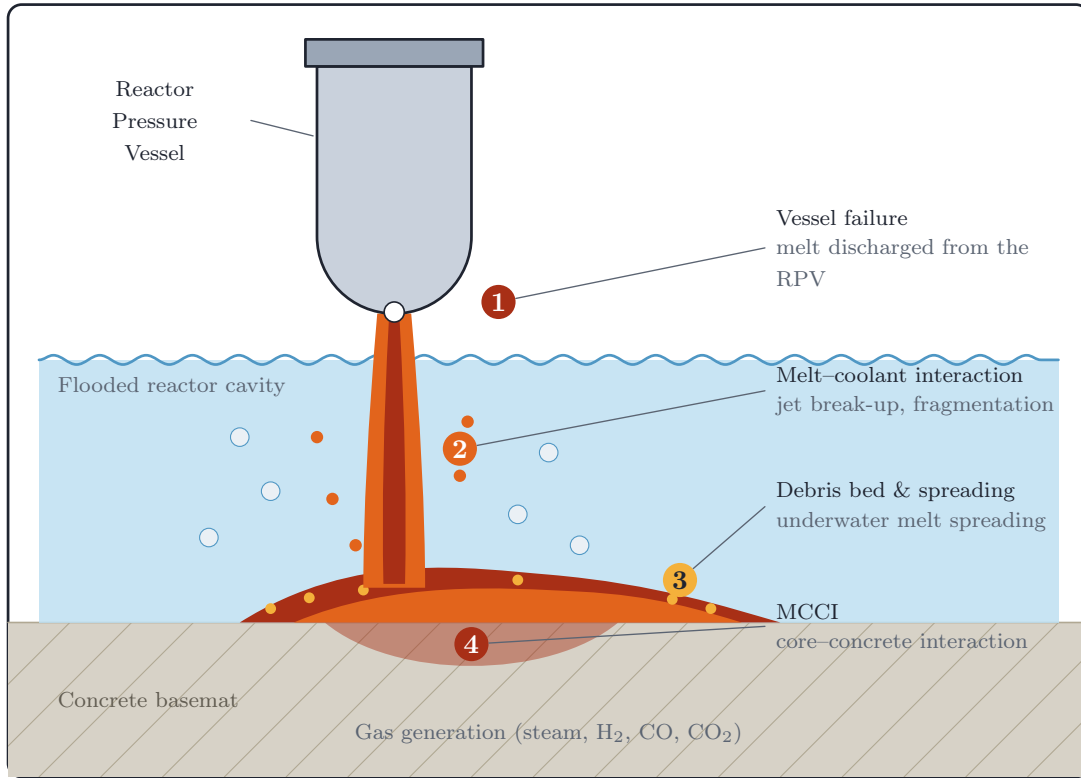


Figure 1.1: Schematic representation of an ex-vessel severe accident scenario following reactor pressure vessel failure.

In this framework, the Nuclear Regulation Authority (NRA) of Japan, in collaboration with the Royal Institute of Technology (KTH) in Sweden, launched the *Molten Core Cooling Phenomena* research programme. The programme was designed to address key uncertainties related to severe accident mitigation, with particular attention to the behaviour and coolability of molten core material after vessel failure [14].

1.2. Experimental research framework

The experimental campaign focused on four main phenomena [14]:

- Melt-vessel interactions, vessel failure, and melt ejection;
- Debris bed formation during melt-coolant interaction;
- Remelting of multi-component debris;
- Liquid melt spreading in shallow water pools.

These phenomena are strongly interconnected, since the way molten material is released, fragmented, spread, and eventually accumulated determines the final debris configuration

and its potential coolability. Within the Molten Core Cooling Phenomena programme, three main experimental facilities were developed: REMCOD, DEFOR, and PULiMS. Each facility was dedicated to a specific part of the severe accident sequence, as summarised in Table 1.1 and schematically illustrated in Figure 1.2.

Table 1.1: Overview of the main experimental programmes within the Molten Core Cooling Phenomena research framework [14].

Programme	Main phenomenon	Relevance for severe accident analysis
REMCOD	Remelting of multi-component debris.	Investigation of melt penetration into porous debris beds and interaction with structural components.
DEFOR	Debris formation during melt-coolant interaction.	Characterisation of particle size distribution, porosity, agglomeration, and debris bed morphology.
PULiMS	Pouring and underwater liquid melt spreading.	Analysis of melt spreading dynamics, final spread area, and melt layer thickness in shallow water.

The *REMCOD* experiments investigated the interaction between hot molten material and pre-existing solid debris or structural components. Their objective was to analyse melt penetration into porous media and to evaluate the influence of parameters such as debris temperature, melt superheat, and capillary effects [14].

The *DEFOR* programme focused on the formation of particulate debris beds during melt-coolant interaction. This topic is relevant because debris bed properties, such as particle size, porosity, agglomeration, and bed geometry, strongly influence water ingression and long-term coolability [14]. In particular, the DEFOR-A experiments quantified the fraction of agglomerated debris as a function of the water pool depth [16], and the formation and cooling of high-temperature debris beds have been investigated both experimentally and analytically within the same research framework [7].

The *PULiMS* programme was dedicated to liquid melt spreading in shallow water pools. The final spread area and layer thickness are important because they determine the surface available for heat removal and influence the possibility of preventing or mitigating MCCI. The main objectives of the PULiMS tests were to measure the spreading dynamics, estimate the front velocity, determine the final spread thickness, and assess the influence of melt temperature and water depth [14]. For this thesis the PULiMS programme is the reference experimental framework.

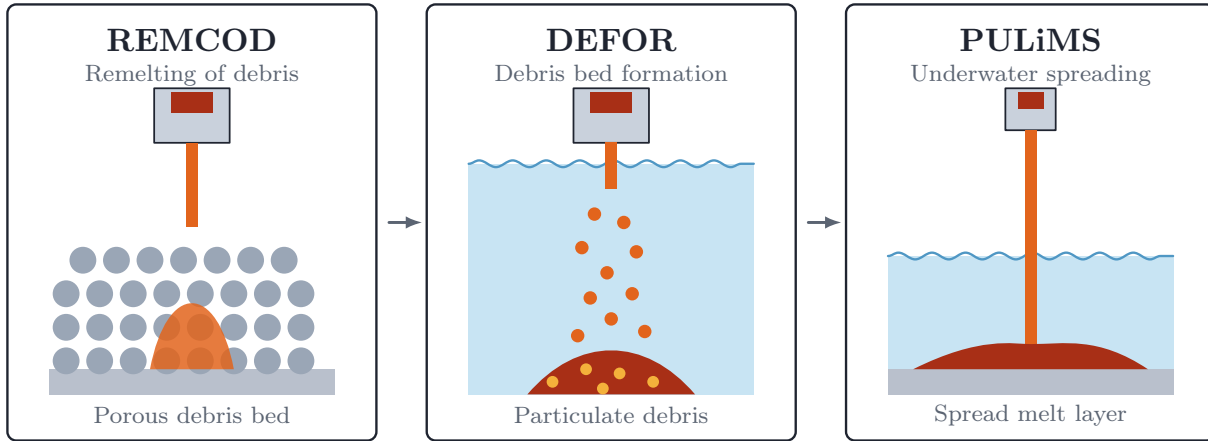


Figure 1.2: Conceptual schematic of the three experimental facilities developed within the Molten Core Cooling Phenomena programme – REMCOD, DEFOR and PULiMS – and of the corresponding melt–coolant configurations, based on [14].

1.3. The PULiMS-E10 experiment

The present work focuses on the PULiMS-E10 experiment. This test is particularly suitable for numerical analysis because it provides experimental information on melt release, underwater spreading, temperature evolution, and final debris bed geometry. Compared with previous PULiMS configurations, the E10 test included improved optical access and a higher spatial resolution of temperature measurements [14].

In the E10 configuration, quartz-glass windows allowed the melt progression to be recorded by multiple video cameras. In addition, the size of the water pool was reduced while preserving the number of installed thermocouples, thus increasing the spatial resolution of the temperature measurements. These features make the experiment a valuable benchmark for the assessment of numerical models devoted to underwater melt spreading.

The main operating conditions of the experiment include a $\text{Bi}_2\text{O}_3\text{--WO}_3$ eutectic simulant, a nozzle diameter of 20 mm , a melt free-fall height in air of 90 mm , a total melt release duration of 17 s , and an initial water temperature of 90°C [14]. The whole experimental test conditions are reported in detail in Chapter 2.

The experimental data available for PULiMS-E10 include the melt delivery rate, selected thermocouple histories, melt front reconstruction from video recordings, and post-test debris bed measurements. These quantities provide the basis for the numerical comparison performed in the present thesis.

1.4. Numerical modelling of melt spreading

Experimental data are essential for understanding underwater melt spreading, but they do not give complete access to all the flow quantities. In particular, the internal velocity field, the transient interface morphology, the local phase distribution and the evolution of the melt accumulation are difficult to measure directly. Computational Fluid Dynamics (CFD) can complement the experimental observations by providing a detailed, time-resolved description of the spreading process [12]. The numerical simulation of underwater melt spreading is, however, challenging, since it combines multiphase flow, large density differences, free-surface deformation, heat transfer, film boiling, cooling-induced viscosity increase, partial solidification and debris formation; a model resolving all these effects at once would require a very complex physical description and a high computational cost [28].

The numerical modelling of corium and melt spreading has a long history in severe-accident research. Early studies relied on dedicated shallow-layer spreading codes, assessed against ex-vessel spreading experiments such as the VULCANO tests [10]. More detailed CFD descriptions were introduced later: Ye et al. [26] simulated the spreading and heat transfer of ex-vessel core melt over the cavity floor, while Kucala et al. [15] developed a computational model coupling free-surface spreading with solidification. A feature common to these spreading models is that the thermal state of the melt is described by a single (mixture) energy equation, and the progressive immobilisation of the melt is reproduced through a strongly temperature-dependent viscosity, frequently based on the Ramacciotti correlation for corium melts [21].

The configuration most relevant to the present work – a melt released into a shallow water pool – has been studied mainly within the KTH and NRA research programmes. Konovalenko and Kudinov [13] proposed a scaling approach to predict the terminal spread thickness of a melt poured into a water pool, whereas the more recent numerical efforts have adopted meshless methods. Zhao [27, 28] simulated melt underwater spreading and infiltration with the Moving Particle Semi-implicit (MPS) method, including a film-boiling heat-transfer model, and Kikuchi et al. [11, 12] reproduced the PULiMS-E10 test with the two-dimensional shallow-water code MSPREAD, coupled to a molten-jet-quench model.

Closely related is the modelling of molten-jet breakup and fuel–coolant interaction, where the Volume of Fluid (VOF) method is frequently combined with a solidification model. Zhou et al. [29] simulated the breakup, cooling and solidification of a metal jet in water, and Liu et al. [18] coupled a VOF method with a solidification model for low-velocity jet breakup; Eom et al. [5] examined the influence of the melt viscosity on corium jet breakup, and Yakush et al. [25] modelled the complementary configuration of a water jet plunging

into a molten heavy-metal pool. These studies confirm that a VOF representation coupled with a temperature-dependent rheology is a suitable and widely adopted framework for melt–coolant interaction problems, and they support the modelling choices made in the present work. The melt immobilisation, in turn, can be described either explicitly, through an enthalpy-based phase-change formulation [23], or implicitly, by letting the viscosity grow with the solid fraction until the melt effectively stops flowing; the latter, computationally lighter route is the one adopted here.

A feature shared by essentially all the CFD and VOF approaches mentioned above is that the thermal field is described by a single energy, or temperature, equation for the melt–coolant mixture. As discussed in detail in Chapter 3, when such a formulation is combined with a sharp-interface VOF representation, the averaging of the melt and water temperatures within the interfacial cells can introduce a spurious cooling of the melt during its fall through the pool. To avoid this artefact, the present work describes the thermal field with two separate transport equations, one for the melt and one for the water temperature, while neglecting the vapour phase. This two-temperature treatment, coupled with the Ramacciotti viscosity law, is the main modelling contribution of the thesis.

Within this context, the present thesis adopts a deliberately simplified CFD approach: the aim is not to reproduce every microscopic phenomenon of the melt–coolant interaction, but to capture the dominant features of the spreading process and to assess how the cooling-induced rheological evolution of the melt affects the final distribution of the material. The numerical model is developed in Simcenter STAR-CCM+ and is based on a transient three-dimensional multiphase formulation. The water–melt interface is described through the Volume of Fluid method, while the thermal behaviour is represented by the two-temperature model, whose melt temperature controls the melt viscosity. The resulting framework provides a computationally affordable tool for comparing the main numerical outcomes with the experimental trends. The overall methodology adopted in this thesis, from the experimental reference data to the comparison between numerical and experimental results, is summarised in Figure 1.3.

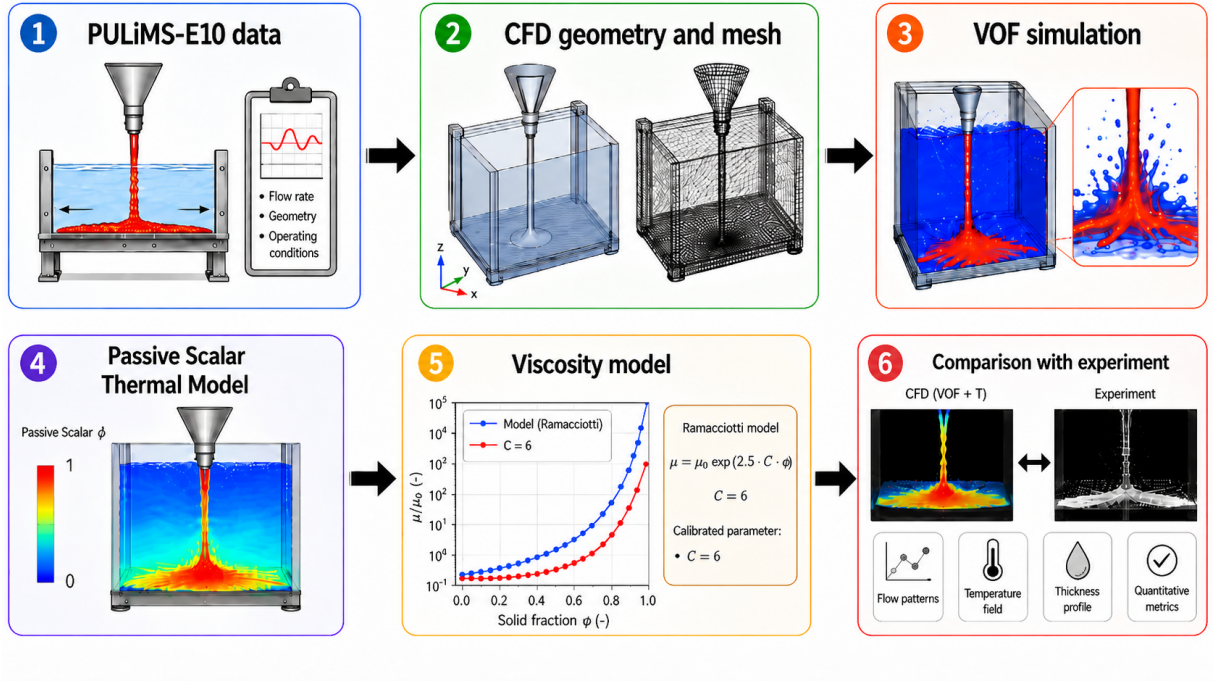


Figure 1.3: Workflow of the thesis methodology.

1.5. Thesis objective

The objective of this thesis is to develop and assess a CFD model of the PULiMS-E10 experiment, with particular attention to the underwater spreading of the $\text{Bi}_2\text{O}_3\text{--WO}_3$ melt and to the final accumulation of the material on the bottom plate.

The work is structured around four main objectives:

- Reproduce the main geometrical and operating features of the PULiMS-E10 experiment in a simplified numerical domain;
- Simulate the transient propagation of the melt in the water pool using a Volume of Fluid approach;
- Introduce a two-temperature melt–water heat-exchange model and a temperature-dependent viscosity model;
- Compare the numerical results with the available experimental data in terms of melt front propagation, spreading behaviour and debris bed geometry.

The thesis also aims to clarify the capabilities and limitations of the proposed modelling strategy. The model is intended to reproduce the macroscopic spreading behaviour of the melt, but it does not explicitly resolve all phenomena occurring in the experiment,

such as detailed boiling dynamics, melt fragmentation, crust rupture, or the formation of a porous debris bed. These limitations are discussed in detail in Chapter 3 and in the interpretation of the numerical results in Chapter 4.

The overall purpose of the work is therefore to evaluate whether a simplified but physically motivated CFD methodology can provide useful insight into underwater melt spreading and support the interpretation of the PULiMS-E10 experimental observations.

2 | PULiMS E-10 Experiment

This chapter focuses on the PULiMS-E10 test, the experimental case examined in the present study. The purpose is to provide a clear and comprehensive description of the reference experiment adopted for the numerical investigation. Within the PULiMS experimental campaign, the E10 test represents a particularly relevant case, since it investigates melt spreading in a shallow water pool and was performed under modified geometric and operating conditions with respect to the previous tests carried out in the same facility. These changes were introduced to improve the observation of the transient spreading process and to increase the amount of useful information gained from the test [14].

In particular, with respect to the previous experiments, the test section was equipped with quartz-glass windows that allowed the melt progression to be recorded by multiple video cameras, thus providing a more detailed visualisation of the phenomenon. Moreover, the size of the water pool was reduced by half while preserving the same number of installed thermocouples: this increased the spatial density of the sensors and, consequently, the spatial resolution of the temperature measurements. At the same time, the melt supply rate was increased consistently with the modified pool geometry [14].

As a result of these features, the PULiMS-E10 experiment is a valuable benchmark for the analysis of melt spreading dynamics and for the assessment of the numerical model developed in this work.

2.1. Experimental setup

The PULiMS facility consists of several main components, including a 45 kW power generator, an induction furnace equipped with a SiC crucible, a melt delivery funnel terminating in a nozzle, a melt spreading pool, the supporting structural frame, and a total of 86 thermocouples. The generator supplies power to the induction furnace, where the melt is produced and heated inside the SiC crucible. The molten material is then discharged through the delivery funnel and released through the nozzle into the spreading pool. The structural frame provides mechanical support to the entire facility, while the

thermocouples allow continuous monitoring of the thermal evolution of the system during the experiments [14].

A scheme of the experimental setup is shown in Figure 2.1.

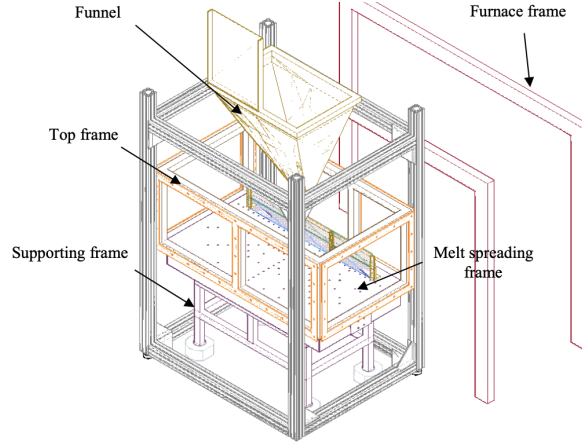


Figure 2.1: PULiMS-E10 (N4) test setup - general view. [14]

The PULiMS-E10 test section consists of an open stainless-steel container with dimensions of 0.8 m in height, 1.6 m in length, and 0.9 m in width, positioned 0.9 m above the ground on the supporting frame. The lateral walls are made of 10 mm thick transparent plexiglass to enable direct visualisation of the melt spreading process, and they are sealed to the upper frame. The melt spreading plate is a 10 mm thick stainless-steel structure provided with multiple feedthroughs for the installation of thermocouples used for temperature measurements. On the rear side of the spreading plate, a set of quartz glass panels is installed, while the melt is released near the centre of the facility, at a distance of 15 mm from the glass panel [14].

The nozzle outlet is located 0.29 m above the melt spreading plate and 0.09 m above the water level, corresponding to a melt free-fall height in air of 90 mm, and the melt release is controlled by a plug mechanism specifically designed to prevent melt blockage phenomena. In addition, to detect possible undesired steam explosion events, the facility is equipped with dynamic force sensors, one installed on each leg of the supporting structure.

A more detailed view of the experimental setup is shown in Figure 2.2.

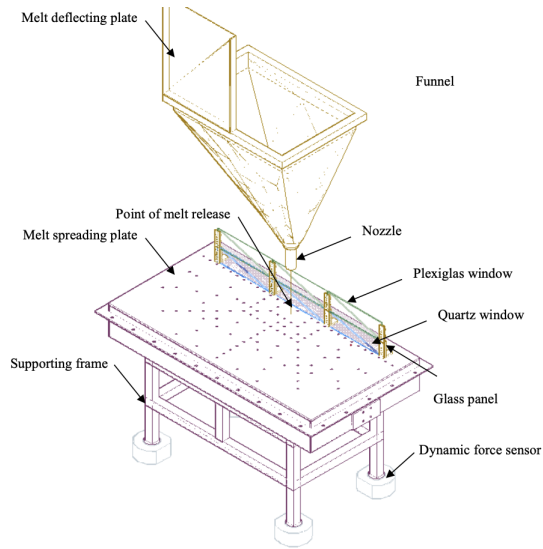


Figure 2.2: PULiMS-E10 (N4) - detailed view. [14]

2.2. Experimental procedure

The experimental procedure begins with the positioning of the crucible inside the induction coil. To minimise heat losses, the gap between the furnace and the induction coil is filled with heat-insulating bricks. The assembly is then covered at the top with a ceramic plate featuring a circular opening to accommodate the crucible and all components are sealed using high-temperature cement, with the aim of reducing convective heat losses around the crucible [14].

The initial charge consists of a mixture of pure Bi_2O_3 and WO_3 powders, prepared according to the eutectic composition, which is the specific proportion of the two oxides that melts and solidifies at a single, well-defined temperature – the lowest of the whole composition range – so that the mixture behaves like a pure substance rather than melting over a temperature interval. In this configuration the liquidus and solidus temperature coincide. This mixture is loaded into the crucible, and its temperature is monitored by thermocouples installed within the crucible. The melting process requires approximately 5 to 6 hours to be completed [14].

A few hours before melt release, approximately 0.28 m^3 of water at 90°C is introduced into the test section to preheat the metallic structures of the facility. Immediately before the experiment, this water is drained and replaced with fresh hot water to ensure well-defined initial thermal conditions [14].

The melt is released once the desired superheat is reached, namely about 39.2°C above the

melting point, giving $T_{melt} = 909.2\text{ }^{\circ}\text{C}$, as measured by the thermocouples in the crucible. During discharge, the molten material first accumulates within the delivery funnel; once the crucible is emptied, the plug mechanism is activated, allowing the melt to exit through the nozzle and enter the test section [14].

After the experiment, the water is drained from the test section and the resulting debris bed is analysed using a laser scanning system to characterise its geometry and morphology [14].

A total of 86 thermocouples were installed in the facility, 80 of which were embedded in the spreading plate to monitor the melt temperature and the dynamics of the spreading process [14]. The spatial distribution of the thermocouples is shown in Figure 2.3.

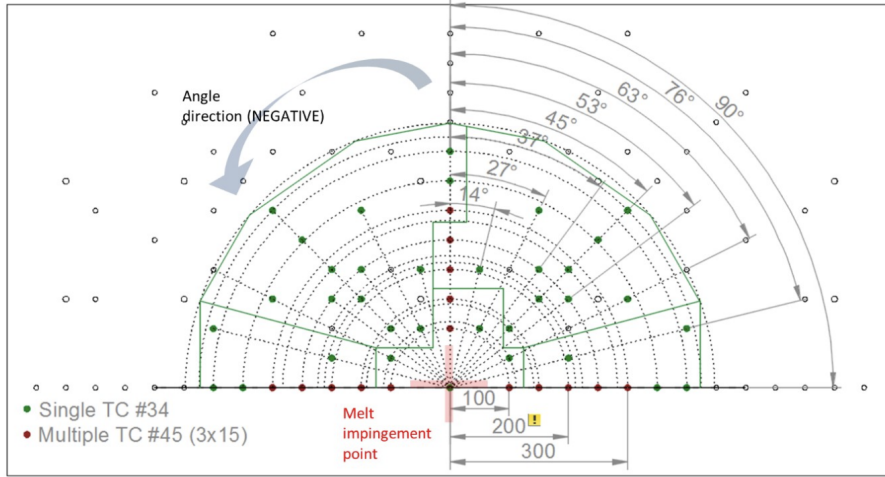


Figure 2.3: TCs locations in the spreading plate. [14]

PULiMS-E10: Summary of the Experimental Procedure

1. Crucible preparation

Crucible positioning inside the induction coil

Thermal insulation with bricks, ceramic plate, and high-temperature cement

2. Melt preparation

Loading of eutectic $\text{Bi}_2\text{O}_3\text{--WO}_3$ powder mixture

Melting and temperature control for approximately 5–6 h

3. Test section preheating

Injection of 0.28 m^3 of water at 90°C

Drainage and replacement with fresh hot water before pouring

4. Melt release

Superheated melt accumulation in the delivery funnel

Plug opening and discharge through the nozzle into the test section

5. Post-test operations

Water drainage from the test section

Laser scanning of the debris bed geometry and morphology

2.3. Test conditions

The main test conditions of the PULiMS-E10 experiment are summarised in Table 2.1.

Parameters	PULiMS-E10	Units
Melt characteristics:		
Simulant material	Bi ₂ O ₃ –WO ₃	-
Melt composition	27-73	%mol
Melt composition	43-57	%mass
Melt characteristics	eutectic	-
Liquidus Temperature	870/1143	°C/K
Solidus Temperature	870/1143	°C/K
Estimated theoretical density of solid mixture	7838	kg/m ³
Estimated theoretical density of melt at $T_{\max}$	6835	kg/m ³
Max melt temperature in the nozzle	909.2/1182.2	°C/K
Melt superheat in the nozzle	39.2	°C
Melt delivery:		
Nozzle diameter	20	mm
Melt free fall height in air	90	mm
Total duration of melt release	17	s
Water pool:		
Dimensions (LxWxH)	1.6x0.9x0.2	m
Temperature	90/363	°C/K
Subcooling	10	°C

Table 2.1: PULiMS-E10 test conditions. [14]

2.4. Results outline

The most relevant results obtained from the experiment concern the characterisation of melt behaviour and debris formation under the considered operating conditions. The results analysed are:

- Melt mass delivery rate.
- Melt and water temperatures.

- Melt spreading.
- Debris bed geometry and morphology.

2.4.1. Melt release

To determine the melt delivery rate, three force sensors were placed beneath the supporting frame of the funnel, enabling continuous measurement of the melt mass accumulated inside the funnel.

The resulting melt mass delivery rate is reported in Figure 2.4. Since the sensor signals were influenced by oscillations of the supporting structure, a moving-average filter was applied to the raw measurements to reduce noise (red line) and obtain a smoother trend (green line).

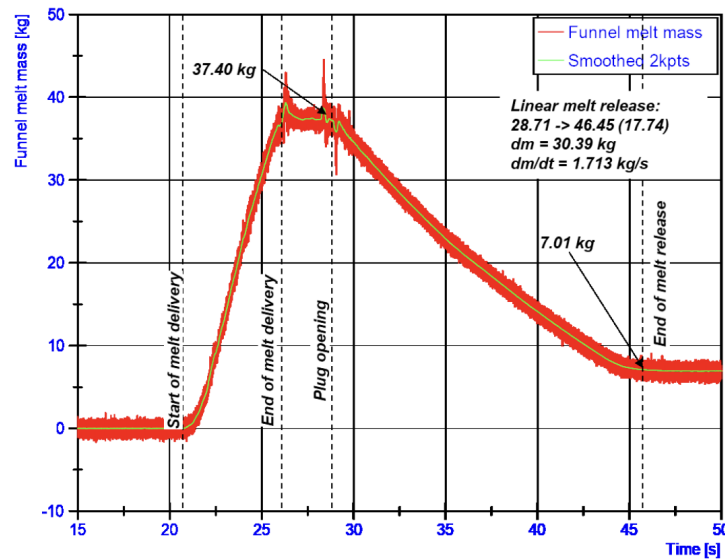


Figure 2.4: PULiMS-E10 (N4) melt delivery rate. [14]

2.4.2. Melt and water temperature

This section presents the temperature measurements recorded during the experiment, with particular focus on the thermocouples installed in the spreading plate. Although temperature data were collected from all 86 thermocouples, only 6 representative sensors are discussed here for the sake of clarity and readability. The nomenclature adopted for the identification of the thermocouples is reported in Table 2.2, while the corresponding temperature histories of the selected thermocouples are shown in Figure 2.5. Following this convention, each sensor is identified by its radial distance from the plate centre, its angular position and the height of its junction above the plate. The six representative

thermocouples discussed here, all at a junction height of 5 mm, are TR000A000H005 (the central sensor), TR100A000H005 and TR200A000H005 (along the 0° direction), TR100A090H005 and TR200A090H005 (along the 90° direction) and TR141A045H005 (on the diagonal). In particular, the central sensor TR000A000H005 is the first to be reached by the melt at the impact point; for brevity it is also referred to as TC0 in the remainder of the thesis, and in Chapter 4 in particular, where it is used as the reference for the impact-zone temperature.

Table 2.2: Designation of TCs located on the melt spreading plate

TRxxxAyyyHzzz	Complete name, where <i>xxx</i> , <i>yyy</i> and <i>zzz</i> define TC position
xxx	Distance from the centre of the spreading plate to the location of the TC (Radius), [mm]
yyy	Azimuthal direction (angle measured clockwise, zero corresponds to the y-axes), [deg]
zzz	Height of the TC junction from the spreading plate, [mm]

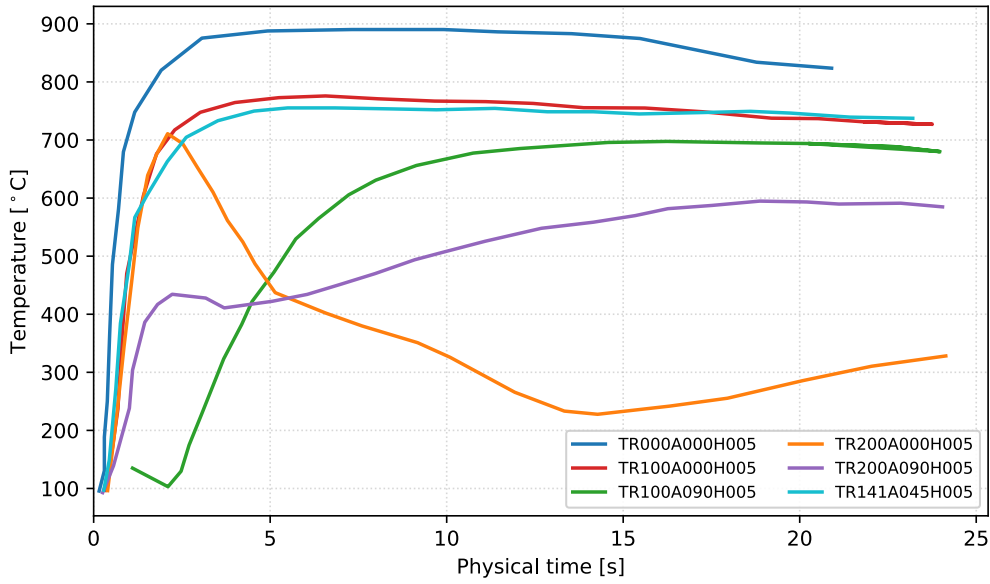


Figure 2.5: Temperature histories recorded by the six representative thermocouples on the spreading plate. Data from [14].

2.4.3. Melt spreading

After the test, the melt spreading process was reconstructed by combining video recordings and thermocouple measurements. High-speed camera images provide a more accurate

estimate of the time at which the melt front reaches specific locations than thermocouple signals. In fact, the K-type thermocouples are not always suitable for determining precise arrival times, owing to their finite response time (which may reach approximately 250 ms), the uncertainty associated with the thermal contact between the melt and the sensor, and the possible shielding effects caused by vapour bubbles or vapour films [14]. The melt front position reconstructed from the thermocouple signals is reported in Figure 2.6, while the reconstruction obtained from the video recordings is shown in Figure 2.7.

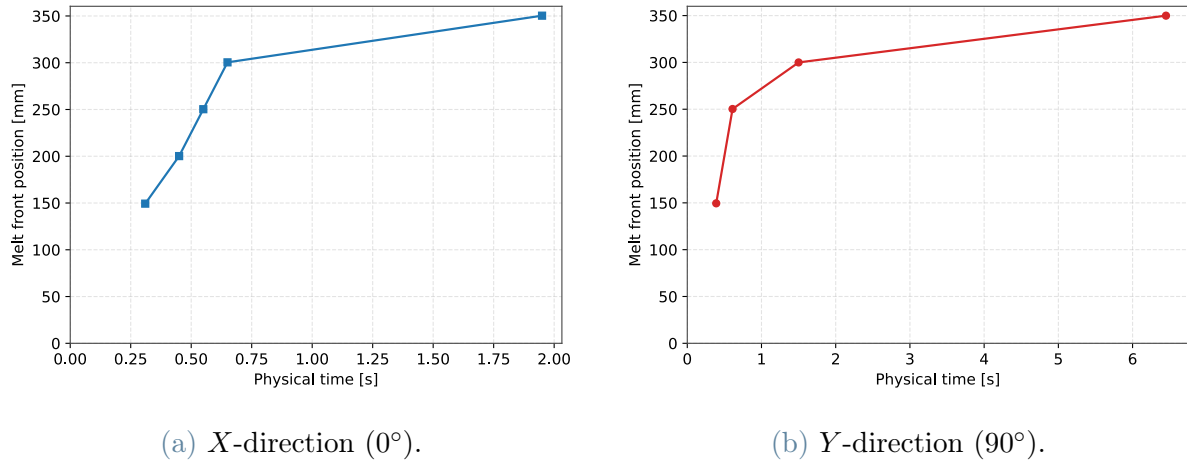


Figure 2.6: Melt front position in the X- (0°) and Y- (90°) directions reconstructed from the thermocouple signals. Data from [14].

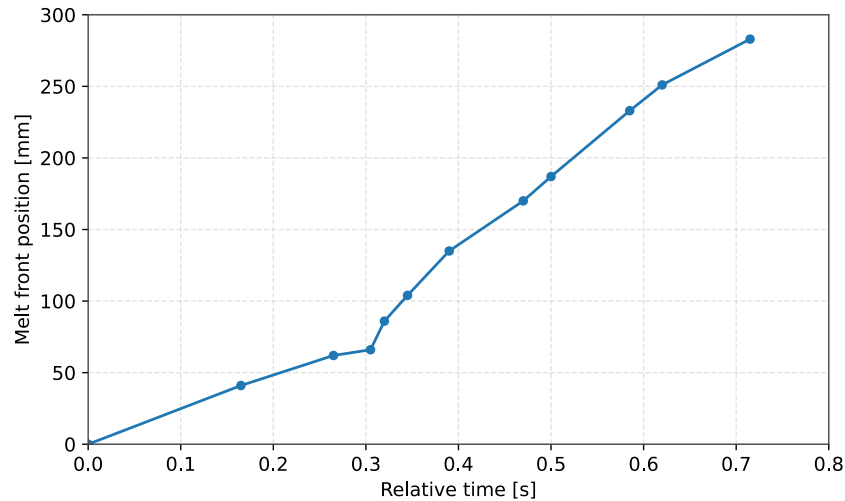


Figure 2.7: Melt front position reconstructed from the high-speed video recordings. Data from [14].

Nevertheless, thermocouples remain an important complementary tool when direct visual

observation is disturbed by aerosols or vapour. This occurs, for instance, in the presence of the so-called “black cloud” generated by fine melt particles suspended in the vapour phase. For this reason, the reconstruction of the spreading process was based on the combined use of both video analysis and thermocouple data [14].

The collected data also indicate that melt spreading may occur in a stepwise rather than fully continuous manner, likely as a consequence of the wave-like propagation of newly arriving melt. A direct comparison between the melt front reconstructed from the thermocouples and from the video recordings is shown in Figure 2.8.

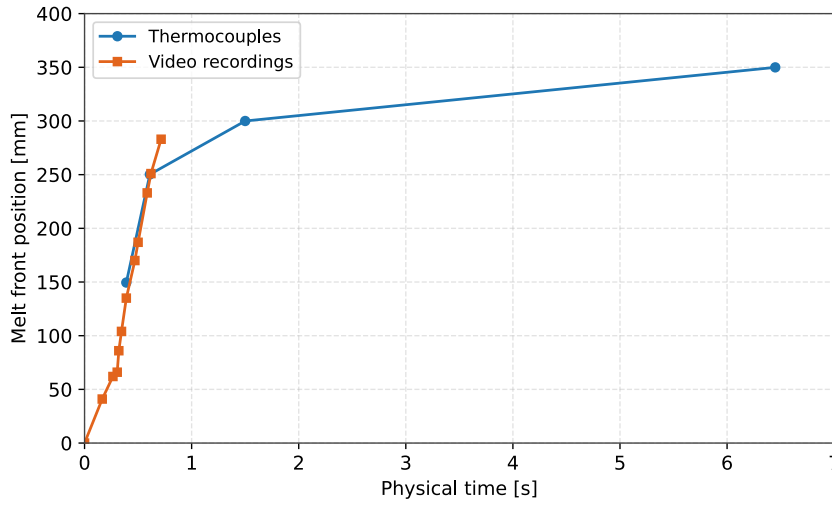


Figure 2.8: Melt front comparison between the reconstruction from the thermocouples (blue) and from the video recordings (orange). Data from [14].

2.4.4. Debris bed geometry and morphology

The relevant geometrical characteristics determined from the laser scans of the debris bed and spreading plate are summarised in Table 2.3.

The solidified debris was found to occupy a moderate fraction of the melt spreading surface. Consistently with previous PULiMS tests, the resulting debris bed was composed of fragmented material, a solidified cake, and localised eruptive structures protruding above the average bed height. Post-test examinations showed that the debris cake exhibited a relatively thick bottom crust, pronounced porosity characterised by elongated voids and channels likely associated with steam and water pathways, and eruptive features interpreted as steam escape channels [14]. The digitised shape of the debris bed obtained from the laser scan is shown in Figure 2.9.

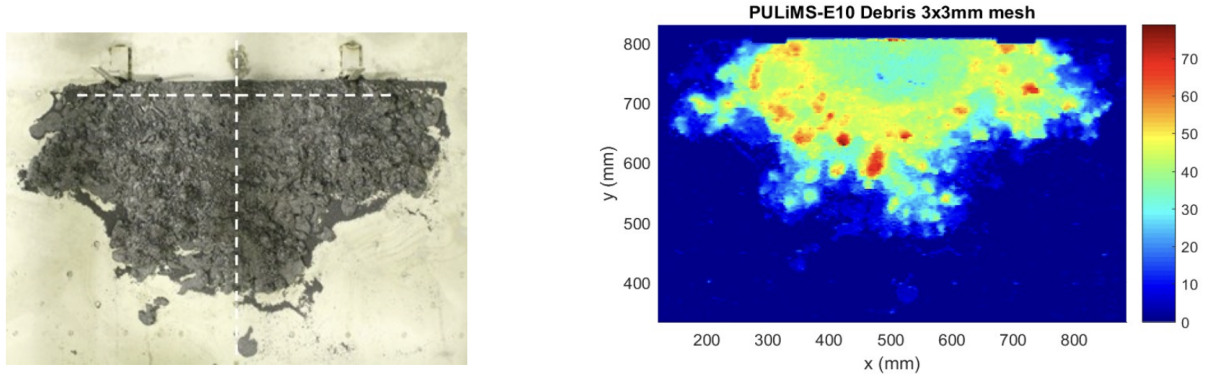


Figure 2.9: Digitised debris bed shape - up view. [14]

Debris bed characterisation	PULiMS-E10	Units
Size along X	729	mm
Size along Y	386	mm
Max height	78.8	mm
Area	0.178	m^2

Table 2.3: Shape scanning results of the debris bed. [14]

2.5. Governing physical phenomena

The phenomena observed in the PULiMS-E10 test are governed by the intense thermal interaction between the high-temperature melt and the subcooled water. Two aspects are particularly relevant for the interpretation of the experiment, and for the modelling presented in the following chapters: the film boiling that surrounds the melt during its fall through the pool, and the nature of the diffuse region observed around the jet impact point.

2.5.1. Film boiling during the melt fall

When a surface whose temperature greatly exceeds the saturation temperature of a liquid is immersed in it, the exchanged heat flux does not increase linearly with the surface superheat $\Delta T_e = T_s - T_{sat}$. The classical boiling curve, reproduced in Figure 2.10, identifies four regimes [1]: free convection, nucleate boiling, transition boiling and film boiling. As the superheat increases, the heat flux rises up to the critical heat flux (point C); beyond it an increasing fraction of the surface becomes blanketed by vapour and the heat flux

decreases, reaching a minimum at the Leidenfrost point (point D). Above this point, in the film-boiling regime, the surface is completely and stably covered by a continuous vapour film that separates it from the liquid bulk.

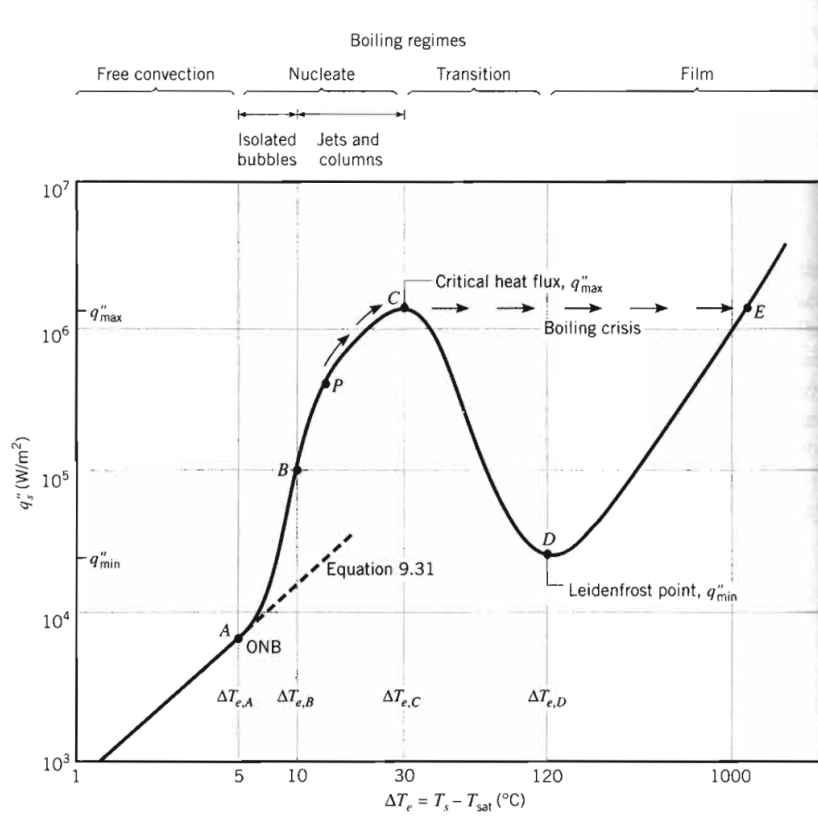


Figure 2.10: Typical boiling curve for water at atmospheric pressure, showing the four boiling regimes and the Leidenfrost point (point D), beyond which the stable film-boiling regime is established [1].

In the PULiMS-E10 test the melt enters the pool at $T_{M,in} \approx 1182\text{ K}$, far above both the saturation and the Leidenfrost temperatures of the water, which at atmospheric pressure corresponds to a wall superheat $\Delta T_e \approx 120\text{ }^\circ\text{C}$ (a surface temperature of about $220\text{ }^\circ\text{C}$) [1]. The falling jet is therefore surrounded by a stable vapour film throughout most of its underwater descent. This film acts as a thermal resistance in series between the melt and the bulk water: since the thermal conductivity of vapour is one to two orders of magnitude lower than that of liquid water, it drastically reduces the effective melt–water heat transfer compared with direct liquid–liquid contact. Film boiling around a falling melt jet is indeed widely recognised as a governing phenomenon of the early stages of fuel–coolant interaction [4]. Once the melt reaches the plate and starts spreading, the compact jet geometry is lost and a continuous vapour film can no longer be sustained, so that direct melt–water thermal interaction becomes physically significant. The two stages

are illustrated schematically in Figure 2.11.

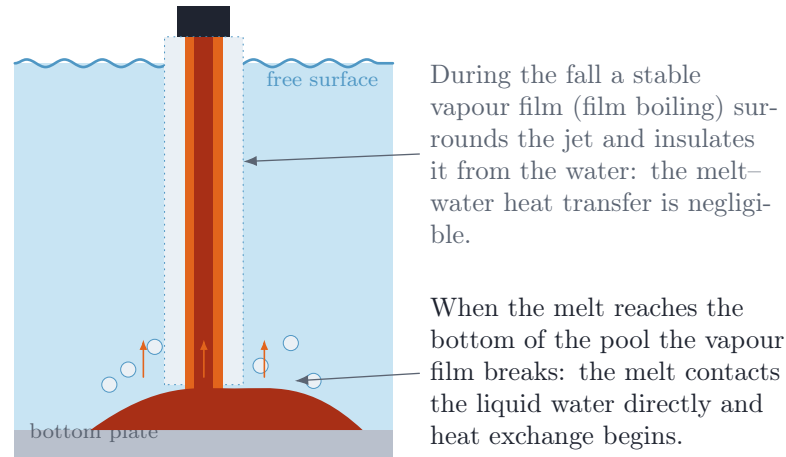


Figure 2.11: Schematic of the film-boiling behaviour of the melt in PULiMS-E10. During its fall the jet is surrounded by a stable vapour film that insulates it from the surrounding water; when the melt reaches the bottom of the pool the film breaks and the melt exchanges heat directly with the liquid water.

2.5.2. The impact region: vapour or solidified melt

The PULiMS-E10 test has also been analysed by Kikuchi et al. [11] with the two-dimensional shallow-water code MSPREAD, which introduces a molten jet quench model for the melt–coolant interaction at jet impingement. In this model (Figure 2.12), the water trapped beneath the impinging jet vaporises and breaks the jet into discrete “melt slugs” of the order of one centimetre; these slugs spread on the floor in a dispersed state while being cooled by the surrounding boiling flow, and eventually coalesce into a porous, three-layer solidified bed. A central element of this picture – and of the original PULiMS reports [14] – is that the diffuse, light-coloured region observed by the cameras around the impact point is interpreted as vapour, which is in turn assumed to drive the fragmentation of the jet.

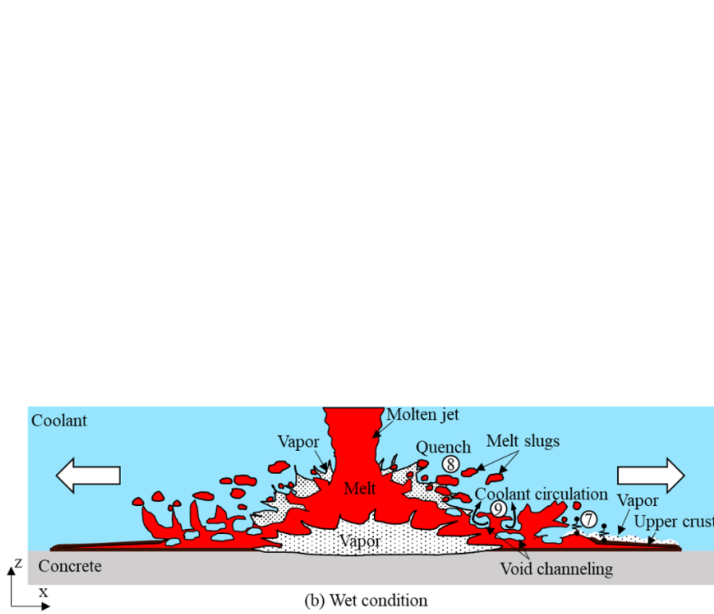


FIGURE 1: CONCEPTUAL ILLUSTRATION OF KEY PHENOMENA OF MELT SPREADING

(a) Key phenomena of underwater melt spreading.

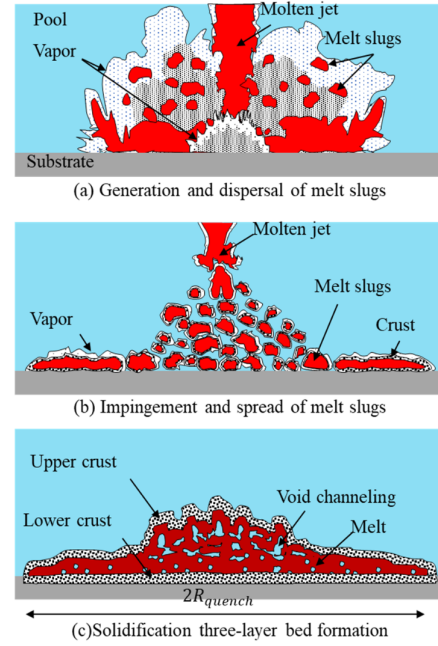
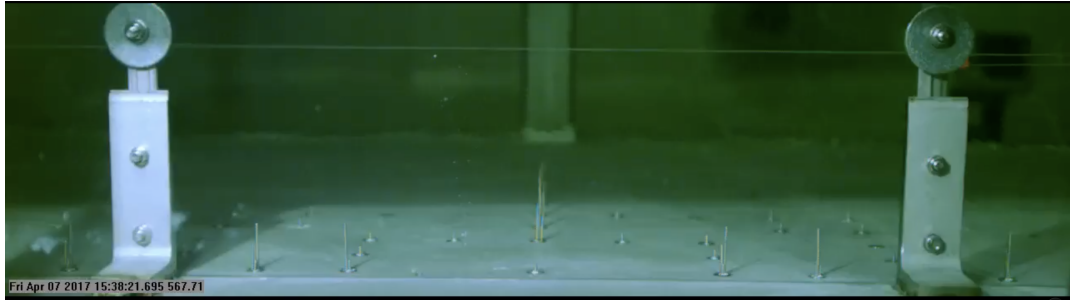


FIGURE 5: THREE-STEP DECOMPOSITION OF QUENCH

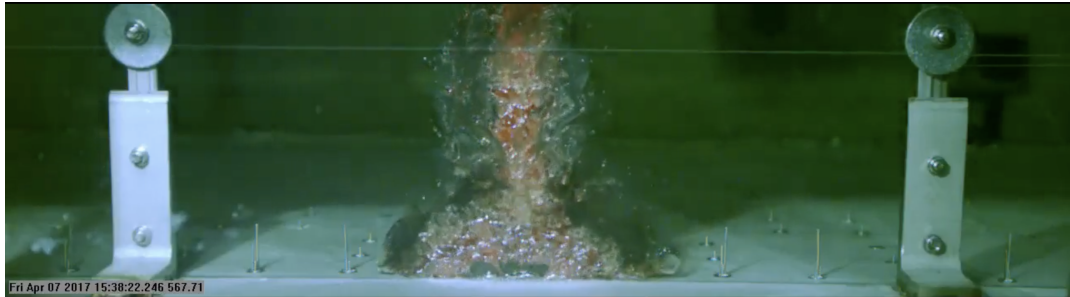
(b) Three-stage molten jet quench.

Figure 2.12: Molten jet quench model proposed for the PULiMS-E10 test: (a) conceptual illustration of the key spreading phenomena and (b) the three-stage decomposition of the quench process [11].

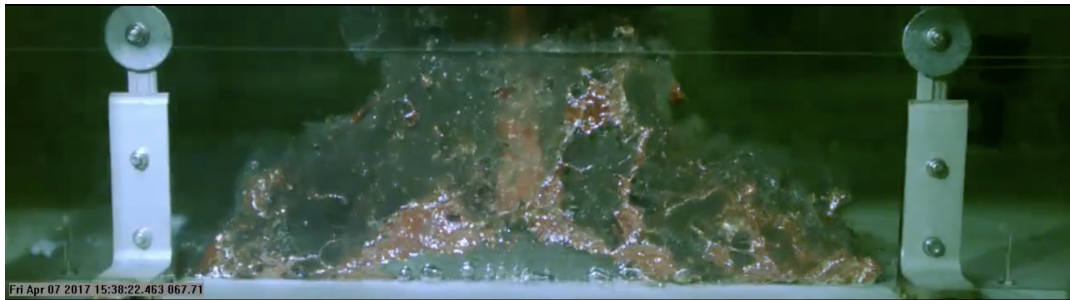
A closer inspection of the original high-speed recordings (Figure 2.13) suggests a different interpretation of that region. Rather than vapour, the diffuse cloud surrounding the impingement point is here interpreted as melt that has already undergone rapid surface solidification and local accumulation upon contact with the subcooled water and the spreading plate. The two phenomena produce a visually similar light-coloured cloud, but they correspond to different physical mechanisms: a vapour-driven, fragmentation-dominated process in the first interpretation, and a thermal/rheological, solidification-dominated process in the second.



(a) Before melt arrival: spreading plate with the thermocouple array.



(b) Jet impact: diffuse, light-coloured region at the impingement point.



(c) Melt spread over the bottom plate.

Figure 2.13: Selected high-speed video frames of the PULiMS-E10 test, showing the evolution of the impact region from melt arrival to the final spreading stage [14].

It must be said that this interpretation rests on visual inspection of the recordings rather than on independent instrumented evidence. It is, however, physically consistent with the two-stage picture described above: during the fall the jet is insulated by the vapour film, whereas once the melt reaches the bottom and the film breaks down, the melt comes into direct contact with the surrounding subcooled water and is rapidly cooled. Under this reading, the diffuse cloud observed around the impingement point is dominated by the rapid surface solidification and local accumulation of the melt, rather than by a sustained vapour layer driving its fragmentation.

3 | CFD Modeling

This chapter presents the numerical methodology adopted to reproduce the PULiMS-E10 experiment using Simcenter STAR-CCM+. The objective of the simulation is to describe the main features of underwater melt spreading, with particular attention to the melt front propagation, the final spreading extent, and the role of cooling-induced viscosity increase.

3.1. Introduction to the CFD Modeling and Strategy

The simulation was developed as a three-dimensional, transient, multiphase model based on the Volume of Fluid (VOF) method. The two phases considered in the model are water and $\text{Bi}_2\text{O}_3\text{--WO}_3$ melt. The VOF approach allows the interface between the two immiscible fluids to be captured through the local phase volume fractions.

A key modelling choice of the present work concerns the treatment of the thermal field. Instead of solving a single energy equation for the melt–water mixture, the model solves two separate transport equations for the temperature, one for the melt and one for the water phase, while the vapour phase is not represented. This choice was introduced after preliminary simulations performed with the standard mixture temperature model showed an undesired decrease of the melt temperature during the falling stage, even when the effective thermal conductivity was set to zero. The artefact originates from the averaging of the two very different phase temperatures within the VOF interface cells; transporting the two phase temperatures separately avoids this spurious cooling and keeps the hot melt and the cold water thermally distinct across the interface. This treatment is also consistent with the physics of the experiment, where the high-temperature melt falling through the pool is surrounded by a vapour film that strongly limits the melt–water heat transfer during the early falling stage [1, 28].

The melt and water temperatures are transported by their own equations and exchange heat only through a simplified source term, which is activated once the melt has penetrated below a prescribed depth in the pool. In this way the melt temperature is kept

essentially unchanged during the fall and starts to evolve only when the melt approaches the spreading region. The melt temperature is then used to evaluate the equivalent solid fraction and, through the Ramacciotti model, the apparent viscosity of the melt.

The numerical strategy can therefore be summarised as follows: the hydrodynamics of the water–melt system is solved with the VOF method, while the thermal behaviour is described by two phase-temperature transport equations, for the melt and for the water, the vapour phase being neglected. In the code this corresponds to running the flow solver in isothermal mode and carrying the two phase temperatures through dedicated transport equations. Since the melt temperature controls the melt viscosity, and hence enters the momentum balance, it is not a passive scalar in the strict sense, but a temperature field two-way coupled to the flow.

3.1.1. Governing equations and the CFD approach

Computational Fluid Dynamics (CFD) is a numerical methodology used to solve the governing equations of fluid flow and heat transfer over a discretised computational domain. In general, CFD formulations may rely on finite-difference, finite-volume, or finite-element techniques. In the present work, the simulations were performed with *Simcenter STAR-CCM+*, which is primarily based on a *finite volume* formulation for fluid-dynamic applications [22]. This approach is particularly suitable for strongly coupled conservation problems, since mass, momentum, and energy conservation are directly linked.

The governing equations are the following [24]:

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (3.1)$$

Momentum Equation:

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot [\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \rho \mathbf{g} + \mathbf{S}_m \quad (3.2)$$

Energy Equation:

$$\rho c_p \left(\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T \right) = \nabla \cdot (k_{eff} \nabla T) + \mathbf{S}_T \quad (3.3)$$

where:

- $\mathbf{u}$ is the velocity vector;
- p is the pressure;
- ρ is the density;
- μ is the dynamic viscosity;
- c_p is the specific heat capacity;
- k is the thermal conductivity;
- $\mathbf{S}_m$ and $\mathbf{S}_T$ denote additional source terms introduced by specific physical models.

3.2. Volume of Fluid (VOF) model

The melt-water system considered in this work is characterised by the coexistence of two immiscible phases separated by a moving interface. To capture such an interface, the Volume of Fluid (VOF) method is employed. The VOF approach describes the spatial distribution of each phase through a scalar volume fraction transported in time. The governing equations for the VOF model are the following [22]:

Referring to a control volume, the volume fraction of a phase i is:

$$\alpha_i = \frac{V_i}{V} \quad (3.4)$$

For a multiphase system, the balance between the volume fractions is:

$$\sum_i^N \alpha_i = 1 \quad (3.5)$$

Transport equation for the single phases:

$$\frac{\partial \alpha_i}{\partial t} + \mathbf{u} \cdot \nabla \alpha_i = S_{\alpha_i} \quad (3.6)$$

In this formulation, $\alpha_i = 1$ identifies a cell fully occupied by the single phase i , whereas $\alpha_i = 0$ indicates a cell where the single phase i is absent, and $0 < \alpha_i < 1$ an interfacial cell. The interface is therefore not tracked explicitly as a sharp boundary, but reconstructed indirectly through the evolution of the phase fraction field.

The fluids that are present in the same interface cells are treated as a mixture. The

material properties calculated in the interface depend on the material properties of the constituent fluids as follows [22] :

$$\rho = \sum_i^N \rho_i \alpha_i \quad (3.7)$$

$$\mu = \sum_i^N \mu_i \alpha_i \quad (3.8)$$

$$c_p = \sum_i^N \frac{c_{p,i} \rho_i}{\rho} \alpha_i \quad (3.9)$$

Continuity equation for the mixture:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = S_m \quad (3.10)$$

with S_m a mass source term that is related to the phase source term as follows:

$$S_m = \sum_i S_{\alpha_i} \cdot \rho_i \quad (3.11)$$

Accordingly, the momentum equation for the mixture becomes:

$$\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot [\mu(\nabla u + \nabla u^T)] + \rho g + F_b + S_m \quad (3.12)$$

Energy equation:

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho u h) = \nabla \cdot (k_{eff} \nabla T) + \mathbf{S}_T \quad (3.13)$$

3.3. Computational domain and geometrical simplifications

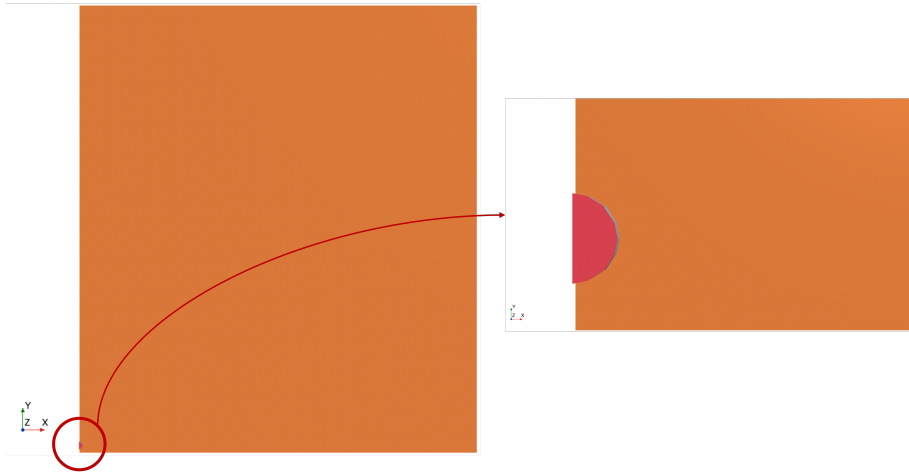
The computational domain was built starting from the main geometrical features of the PULiMS-E10 test section. The experimental configuration consists of a shallow water pool into which the molten $\text{Bi}_2\text{O}_3\text{-WO}_3$ simulant is released through a nozzle. In the

experiment, the nozzle outlet is located above the spreading plate and above the initial water level. The reference test conditions report a nozzle diameter of 20 *mm*, a melt free-fall height in air of 90 *mm*, a total release duration of 17 *s*, and a water pool temperature of 90°C [14].

Several geometrical simplifications were introduced to reduce the computational cost while preserving the main physical features of the spreading process:

- The nozzle was simplified as a short cylindrical inlet region rather than modelling the complete melt delivery system. This approximation neglects the detailed flow development inside the funnel and nozzle, but allows the melt to be injected into the pool with the prescribed inlet velocity and phase composition.
- The in-air free fall of the melt between the nozzle outlet and the water surface is not simulated explicitly. The 90 mm air gap is excluded from the computational domain and the velocity gained during the free fall is imposed directly at the inlet, as detailed in Section 3.7.1. This avoids meshing an air region while preserving the correct melt velocity at pool entry.
- Only half of the pool was simulated by applying a symmetry boundary condition on the central plane, with the inlet mass flow rate correspondingly halved with respect to the experimental value. This is justified by the symmetry of the experimental configuration: the melt is released at the centre of the pool and the spreading is expected to develop symmetrically about that plane, so that simulating one half does not affect the description of the dominant spreading dynamics while approximately halving the number of computational cells and the simulation time.
- The detailed geometry of the experimental support structures, thermocouple feedthroughs, and external components was not included. The numerical domain was limited to the fluid region required to describe melt injection, underwater fall, impact on the bottom plate, and subsequent spreading.

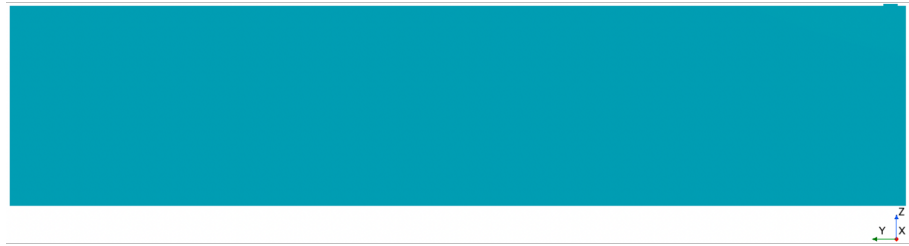
The resulting computational geometry is shown in Figure 3.1, which reports the top view including the nozzle inlet region (Figure 3.1a), the side view of the quartz-glass wall used as optical access in the experiment (Figure 3.1b), and the symmetry wall adopted for the half-domain representation (Figure 3.1c).



(a) Top view of the computational geometry, including the melt inlet/nozzle region.



(b) Side view of the quartz-glass wall used as optical access in the experiment.



(c) Symmetry wall adopted to represent the half-domain configuration.

Figure 3.1: Main views of the computational geometry adopted to reproduce the PULiMS-E10 configuration.

A three-dimensional view of the resulting domain is given in Figure 3.2, which shows the overall shape of the half-pool model.

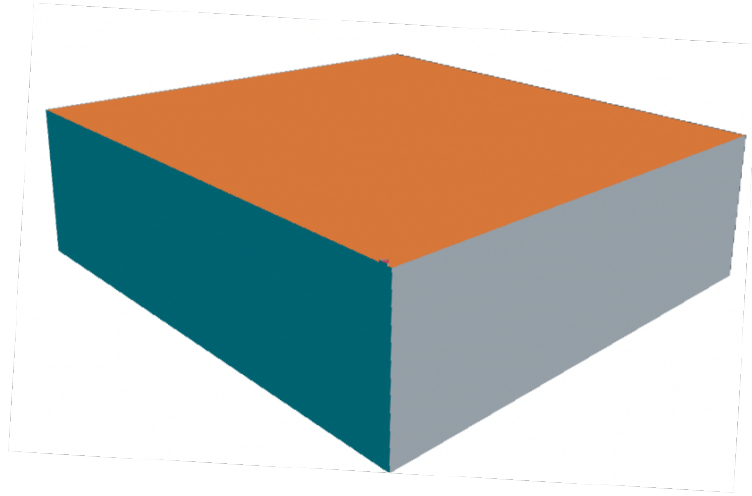


Figure 3.2: Three-dimensional view of the computational domain used in the simulations (half-pool model).

3.4. Mesh generation and adaptive refinement

The computational mesh was generated using the automated mesh workflow available in Simcenter STAR-CCM+. The adopted meshing strategy was based on the surface remesher and the trimmed cell mesher. The surface remesher was used to obtain a high-quality surface discretisation before volume mesh generation, while the trimmed cell mesher was selected because it provides a predominantly hexahedral, Cartesian-dominant mesh that is robust and efficient for general-purpose CFD applications [22, Meshing]. This topology was considered suitable for the present transient VOF simulations, since it allows a regular discretisation of the pool domain and facilitates controlled mesh refinement in the regions where the melt–water interface and the spreading front are expected to evolve.

The computational mesh was generated by defining a global base size and then introducing local refinement in the region where the melt jet enters the water pool. A local volumetric control was introduced in the nozzle and jet impingement region to increase the spatial resolution where the melt enters the water pool and where the first melt–water interaction occurs. This local refinement was therefore used to better resolve the initial jet motion, the impact region, and the early development of the melt–water interface, as shown in Figure 3.3.

Table 3.1: Mesh sizing parameters adopted in the CFD model.

Mesh parameter	Relative value	Absolute value [m]
Base size	100%	0.0260
Target surface size	75% of base size	0.0195
Minimum surface size	5% of base size	0.0013
Local volumetric refinement size	15% of base size	0.0039

The values schematised in Table 3.1 were adopted to control the surface discretisation while preserving a reasonable overall cell count.

In addition to the static mesh refinement, adaptive mesh refinement (AMR) was activated during the transient simulation [22, Adaptive Mesh Refinement]. The AMR strategy was based on the free-surface mesh refinement criterion available in STAR-CCM+, so that the grid could be dynamically refined in cells characterised by strong phase-fraction gradients. In the present VOF simulation, these regions correspond to the water–melt interface. Therefore, the adaptive mesh allowed the resolution to be increased only where the interface dynamics were locally relevant, while preserving a coarser mesh in the bulk water region and in areas not reached by the melt, as can be seen in Figure 3.3.

The adopted adaptive mesh settings are summarised in Table 3.2.

Table 3.2: Adaptive mesh refinement settings adopted in the transient VOF simulation.

AMR parameter	Adopted value
Adaptation mode	Mid-Point Subdivision
Prism cell refinement	None
Initial mesh	General
Transition width	2
Minimum adaptation cell size	5.0×10^{-5} m
Face validity check	Enabled
Minimum face validity	0.9
Free-surface mesh refinement	Enabled
Maximum refinement level	4
Resolution criterion for interface	3.0
Estimated level-4 size from base mesh	1.6×10^{-3} m
Estimated level-4 size from local refined region	2.4×10^{-4} m

The free-surface refinement criterion was enabled with a maximum refinement level equal

to 4, so this means that, in the refined regions, the same cell can be progressively subdivided up to four refinement levels. As an order-of-magnitude estimate, starting from the global base size of 0.026 m, a level-4 refinement corresponds to a local cell size of approximately:

$$\frac{0.026}{2^4} \simeq 1.6 \times 10^{-3} \text{ m.} \quad (3.14)$$

In the statically refined nozzle and impingement region, where the characteristic cell size was already reduced to 0.0039 m, the same refinement factor would correspond to a local cell size of approximately

$$\frac{0.0039}{2^4} \simeq 2.4 \times 10^{-4} \text{ m.} \quad (3.15)$$

These values should be interpreted as indicative local length scales, since the actual cell size depends on the local trimmed-cell topology and on the adaptive refinement history.

A minimum adaptation cell size equal to 5.0×10^{-5} m was also imposed to prevent excessive refinement and avoid the generation of unnecessarily small cells during the transient calculation. Moreover, a transition width equal to 2 was used to smooth the refinement variation between adjacent mesh regions. This setting helps avoid abrupt changes in cell size between the refined interface region and the surrounding coarser mesh. Face-validity checking was kept active, with a minimum face validity equal to 0.9, to preserve acceptable mesh quality during the adaptive refinement process.

The use of AMR therefore represents a compromise between interface resolution and computational cost. A uniformly refined mesh over the entire pool would require a significantly larger number of cells, most of which would be located in regions with limited relevance for the melt spreading dynamics. By contrast, the adopted adaptive strategy concentrates the computational effort near the melt–water interface and the spreading front, where the VOF field changes rapidly and where a higher spatial resolution is required to describe the transient evolution of the melt distribution.

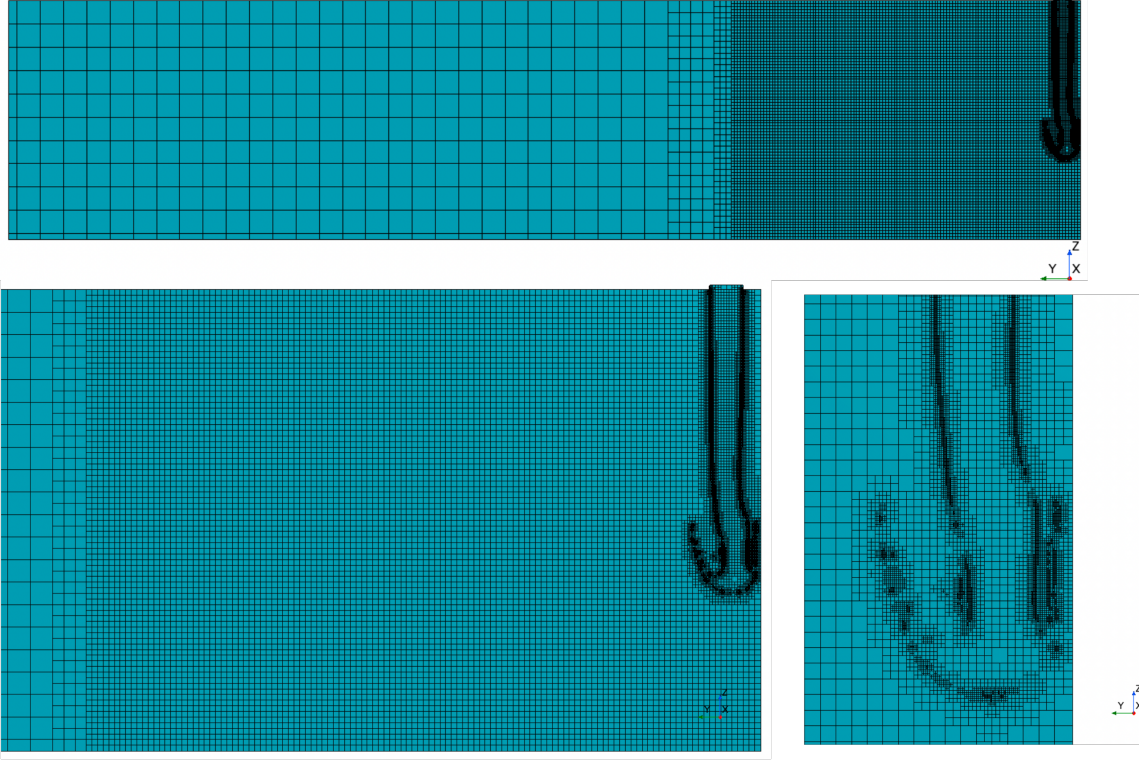


Figure 3.3: Composite view of the computational mesh adopted in the present model. The figure shows: the symmetry-wall view of the computational domain with the overall mesh distribution; an intermediate zoom highlighting the local mesh refinement introduced through the volumetric control; a detailed zoom of the melt jet tip during the falling phase, where the AMR is activated.

3.5. Solver controls and time-step settings

The simulation was advanced in time using an adaptive time-step strategy based on the Courant–Friedrichs–Lewy number. The initial time step was set equal to

$$\Delta t = 5 \times 10^{-4} \text{ s}. \quad (3.16)$$

The CFL-based time-step provider was configured with a target mean CFL number equal to 1 [22]. The minimum allowed time step was:

$$\Delta t_{min} = 2 \times 10^{-4} \text{ s}. \quad (3.17)$$

For each physical time step, 15 inner iterations were performed. The target simulated

physical time was equal to 5 s. This duration was selected to capture the main transient spreading phase after melt injection and impact on the bottom plate.

3.6. Numerical settings: time-step, Courant number, and residual monitoring

All simulations discussed in Chapter 4 were performed using the same mesh generation strategy, adaptive mesh refinement (AMR) settings, and time-step control described in Sections 3.4 and 3.5, so that the relative comparison between cases (e.g. the effect of the Ramacciotti coefficient C or of the activation depth z_{act}) is not affected by inconsistencies in spatial or temporal resolution. This section summarises the numerical indicators that were monitored during the simulations – the Courant number, the adaptive time step and the solver residuals – to check the temporal stability of the time integration, and then discusses the spatial-resolution strategy adopted in the absence of a formal grid-convergence study. These checks should be read as a monitoring of the numerical behaviour of the simulations rather than as a formal demonstration of grid- and time-step independence, which was not within the scope of the present work.

3.6.1. Time-step control and Courant number

As described in Section 3.5, the simulations were advanced using an adaptive time-step strategy based on the Courant–Friedrichs–Lewy (CFL) condition, with a target mean CFL number of 1, an initial time step of 5×10^{-4} s, and a minimum allowed time step of 2×10^{-4} s. Fifteen inner iterations were performed at each physical time step. The evolution of the average CFL number, together with the resulting adaptive time-step size, was monitored throughout each simulation to verify the temporal stability of the time integration, particularly during the most dynamically active phases of the transient – jet impact on the bottom plate and the onset of spreading – where local velocities and phase-fraction gradients are largest.

The temporal discretisation was monitored throughout the reference case (Case 4A). The time step starts from its initial value of 5×10^{-4} s and, within the first instants of the transient, drops to the prescribed minimum of 2×10^{-4} s, at which it then remains for the entire simulation. The domain-averaged Courant number (Figure 3.4a) stays very low throughout, of the order of 10^{-4} , since most of the pool consists of quiescent water and only a small interfacial region around the jet experiences high local velocities; its two mild increases, around $t \approx 0.15$ s and beyond $t \approx 0.6$ s, correspond respectively to the jet

penetration into the pool and to the most active spreading phase.

The maximum Courant number (Figure 3.4b), instead, shows localised spikes during the most dynamic phases of the transient – jet penetration, impact and spreading – reaching high values in a very small number of cells, typically the smallest AMR cells located in the high-velocity jet and impact region. Since the time step is already pinned at its lower bound of 2×10^{-4} s, it cannot be reduced further in those cells. Because STAR-CCM+ advances the flow with an implicit segregated scheme, however, these isolated high-CFL events do not destabilise the solution: the solver residuals do not grow or diverge (Figure 3.5), and the very low domain-averaged Courant number confirms that, away from these few cells, the temporal resolution is conservative. Unlike explicit schemes, for which the time step is restricted by the CFL condition, the implicit time integration adopted here is unconditionally stable and is not subject to that limit [24].

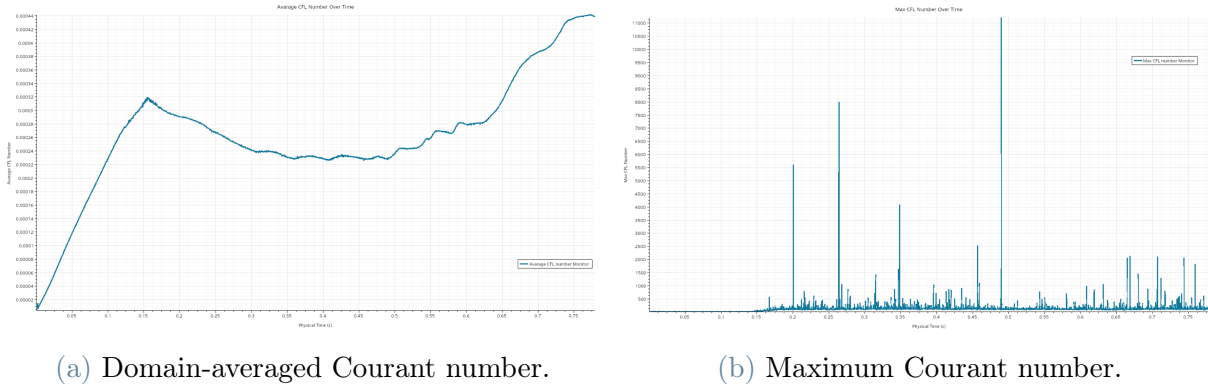


Figure 3.4: Courant-number monitors for the reference case (Case 4A): (a) domain-averaged and (b) maximum Courant number during the simulated transient.

3.6.2. Solver residuals

The convergence of the segregated flow solver at each physical time step was monitored through the residuals of the continuity, momentum, volume-fraction and phase-temperature transport equations. The aim of this monitoring was not to demonstrate a tight convergence within each time step, but to check that the residuals do not grow or diverge as the transient advances, given the fixed number of inner iterations (15 per time step, Section 3.5) used in the simulations.

Figure 3.5 shows a detail of the residual history over a few consecutive time steps. Within each physical time step the fifteen inner iterations reduce the residuals, which then rise again at the start of the next step, when the solution is advanced in time; this saw-tooth pattern repeats from one step to the next. Over the whole simulation the residuals

of the continuity, momentum and volume-fraction equations stay around 10^{-4} – 10^0 and the phase-temperature residual settles at a lower level, without growing as the transient proceeds. This level is relatively high and reflects the strongly transient, multiphase nature of the flow together with the modest number of inner iterations per step: it shows that the time integration does not diverge, rather than that each time step is fully converged.

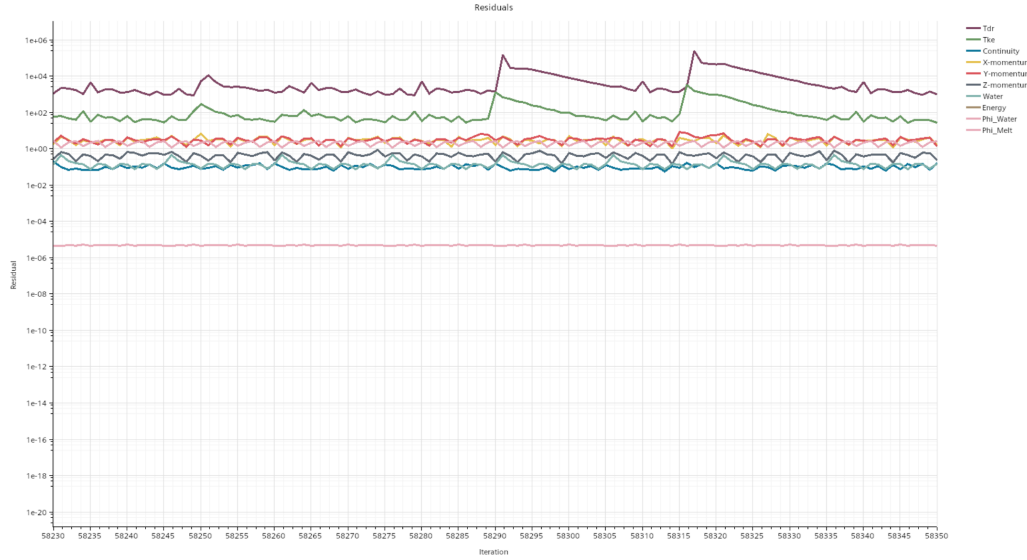


Figure 3.5: Detail of the solver residuals for the reference case (Case 4A) over a few consecutive physical time steps, showing how the inner iterations reduce the residuals within each step.

3.6.3. Mesh resolution and adaptive refinement

A dedicated mesh-independence study, in the sense of a systematic comparison between two or more globally refined meshes run on the same case, was not performed in the present work, primarily due to the high computational cost associated with the transient, AMR-enabled VOF simulations discussed in Chapter 4. Instead, spatial resolution was controlled through the combination of a statically refined volumetric control in the nozzle and jet-impingement region (Table 3.1) and a free-surface-based adaptive mesh refinement (AMR) criterion (Table 3.2), which dynamically concentrates resolution at the melt–water interface as it evolves. This strategy was adopted as a pragmatic alternative to a full grid-convergence study, on the assumption that the interfacial regions – where the volume-fraction gradient is largest – are also the regions most sensitive to spatial resolution, and that the AMR mechanism keeps these regions adequately resolved throughout the transient regardless of the underlying base mesh size.

The qualitative adequacy of this strategy can be appreciated in Figure 3.3 (Section 3.4),

which shows that the adaptive criterion consistently concentrates the finest cells along the melt–water interface during the falling and spreading stages, so that the moving front is always captured by the locally refined grid. It should nonetheless be acknowledged that this approach does not, by itself, demonstrate that the reported results (e.g. the melt front position, or the local accumulation pattern at the impact point) are quantitatively independent of the base mesh size and of the maximum AMR refinement level (set to 4 throughout this work, Table 3.2). A rigorous verification would require repeating at least one reference case with a coarser and a finer base mesh size, while keeping the AMR settings unchanged, and comparing the resulting melt front position and impact-region accumulation. This is left as a recommended extension of the present work and is explicitly listed among the limitations in Section 3.10.

3.6.4. Summary

The numerical behaviour of the simulations was therefore checked through the time-step, Courant-number and residual monitors discussed above. The adaptive time step quickly reaches its lower bound of 2×10^{-4} s, the domain-averaged Courant number stays of the order of 10^{-4} with only localised spikes in a few interfacial cells, and the solver residuals do not grow as the transient proceeds. Taken together, these indicators show that the time integration is stable for the cases analysed in Chapter 4. A formal grid-convergence study was not carried out: the spatial resolution was instead controlled through static local refinement and free-surface adaptive mesh refinement, and a systematic mesh-convergence analysis is left as a recommended extension of the present work (Chapter 5).

3.7. Initial conditions, boundary conditions and material properties

This section collects the problem setup adopted in the simulations: the initial and boundary conditions imposed on the computational domain and the material properties assigned to the two phases.

3.7.1. Initial and boundary conditions

The numerical setup was initialised to reproduce the thermal and mechanical conditions of the PULiMS-E10 test before the beginning of the melt release. The pool was initially filled with water at rest, while the melt was introduced only through the nozzle inlet during the injection stage. The initial water state corresponds to $T_W = 363$ K, whereas

the injected melt is associated with an inlet temperature of $T_M = 1182.2$ K, and the initial pressure field was set equal to the reference pressure of the domain.

The main initial conditions adopted in the simulation are summarised in Table 3.3 [14].

Table 3.3: Initial conditions adopted in the CFD model.

Quantity	Adopted value
Initial water temperature	363 K
Inlet melt temperature	1182.2 K
Initial velocity field	$\mathbf{u} = 0$
Initial pressure field	$p = 0$ Pa gauge

The boundary conditions are reported in Table 3.4.

Table 3.4: Boundary conditions adopted in the CFD model.

Boundary	Condition	Adopted setting
Nozzle inlet	Velocity inlet	$u_{in} = 1.55$ m/s
Top boundary	Pressure outlet	$p = 0$ Pa gauge
Pool walls	Wall	Adiabatic wall
Bottom wall	Wall	Adiabatic wall
Nozzle wall	Wall	Adiabatic wall
Symmetry plane	Symmetry	Simmetry Wall

The melt injection was prescribed through a velocity inlet boundary condition, with the inlet velocity derived from the experimental melt mass flow rate. The upper boundary of the pool was treated as a pressure outlet, all solid surfaces were modelled as impermeable adiabatic walls, and a symmetry boundary condition was applied on the central plane of the pool to reduce the computational domain to one half of the experimental configuration.

The inlet velocity was evaluated in two steps. First, the velocity at the nozzle outlet was obtained from the melt mass flow rate $\dot{m}$, the melt density ρ_M and the nozzle cross-sectional area $A = \pi r^2$ (with nozzle radius $r = 10$ mm):

$$v_0 = \frac{\dot{m}}{\rho_M A} = \frac{1.713}{6835 \cdot \pi \cdot (0.01)^2} \approx 0.8 \text{ m/s.} \quad (3.18)$$

The melt then falls freely in air over the $h = 0.09$ m separating the nozzle outlet from the water surface; the associated velocity increase was accounted for through the free-fall

relation [3], which yields the velocity actually imposed at the inlet:

$$v_{in} = \sqrt{v_0^2 + 2gh} = \sqrt{0.8^2 + 2 \cdot 9.81 \cdot 0.09} \approx 1.55 \text{ m/s.} \quad (3.19)$$

The symmetry condition implies that only half of the pool was simulated; consequently the injected melt mass flow rate is halved with respect to the experimental value, while the inlet velocity (3.19) is preserved. This simplification decreases the computational cost, but it prevents the model from capturing possible asymmetric spreading patterns that may occur in the full experimental domain.

3.7.2. Material properties

The material properties adopted in the CFD model are summarised in Table 3.5. They were selected consistently with the PULiMS-E10 reference conditions and with the simplified thermal formulation implemented in the present work. In particular, the melt was modelled as a $\text{Bi}_2\text{O}_3\text{--WO}_3$ simulant, while water properties were assigned according to the initial pool temperature. The melt density and specific heat capacity were used to define the reference volumetric sensible enthalpy H_0 , whereas the thermal conductivities were used only in the simplified interfacial heat-transfer source term. The reference water temperature was set equal to 363 K, corresponding to the initial pool temperature of the PULiMS-E10 test. The melt inlet temperature was set equal to 1182.2 K, corresponding to the corrected melt temperature at the release nozzle. The liquidus temperature adopted in the model is higher than the nominal eutectic melting temperature of the $\text{Bi}_2\text{O}_3\text{--WO}_3$ mixture: this correction accounts for the change in the melt thermal behaviour caused by the reaction between the simulant and the crucible material during melt preparation, which led to a deviation from the eutectic composition [11].

Table 3.5: Material properties and thermal parameters adopted in the numerical simulation.

Property	Symbol	Value	Unit
Melt properties and parameters			
Melt density [17]	$\rho_M(T)$	$7.896 - 0.001172(T - 273)$	g/cm^3
Melt specific heat capacity [17]	$c_{p,M}$	280	J/(kg K)
Melt thermal conductivity [9]	k_M	5.3	W/(m K)
Melt inlet temperature [14]	$T_{M,in}$	1182.2	K
Solidus temperature [11]	T_{sol}	1143	K
Liquidus temperature [11]	T_{liq}	1189	K
Ramacciotti coefficient	C	4	–
Water properties [19] and interfacial parameters			
Water density	ρ_W	965	kg/m^3
Water specific heat capacity	$c_{p,W}$	4205	J/(kg K)
Water dynamic viscosity	μ_W	0.000315	Pa s
Water thermal conductivity	k_W	0.62	W/(m K)
Reference temperature	T_{ref}	363	K
Surface tension melt–water interaction [17]	σ	0.16	N/m

Note: In the melt density correlation, T is expressed in K.

3.8. Two-temperature thermal model

This section describes the thermal model adopted in this work, in which two transport equations, one for the melt and one for the water temperature, are solved while the vapour phase is neglected. The formulation of the two phase temperatures is presented first, followed by the source term that activates the simplified melt–water heat exchange below the prescribed depth.

3.8.1. Phase-temperature formulation

The two phase temperatures are transported in Simcenter STAR-CCM+ by means of its scalar-transport machinery. A transported scalar is advected and diffused by the flow according to its own conservation equation; in the present work two such scalars are used to carry the normalised sensible enthalpy of the melt and of the water phase, from

which the corresponding phase temperatures are then reconstructed. It is worth stressing that these scalars are not passive in the strict sense: the reconstructed melt temperature controls the melt viscosity and therefore feeds back on the momentum equation, so that the thermal field and the flow are two-way coupled.

The transport equation for a passive scalar component ϕ_i is written in integral form as [22]:

$$\frac{\partial}{\partial t} \int_V \rho \phi_i dV + \oint_A \rho \phi_i \mathbf{v} \cdot d\mathbf{a} = \oint_A \mathbf{j}_i \cdot d\mathbf{a} + \int_V S_{\phi_i} dV, \quad (3.20)$$

where:

- i is the passive scalar component index
- V is the control volume
- $\mathbf{v}$ is the velocity vector
- $\mathbf{j}_i$ is the diffusive flux
- S_{ϕ_i} is the source term associated with the passive scalar component

The thermal evolution of the water–melt system is described by two dimensionless scalars, one associated with the melt phase and one with the water phase, which carry the normalised sensible enthalpy of each phase and from which the two phase temperatures are reconstructed; the vapour phase is not modelled. In the code, the built-in energy model is switched off (isothermal setting) and the heat exchange between the two phases is reproduced through the source term described below.

The main reason for transporting the two phase temperatures separately, rather than solving a single mixture energy equation, is related to the physical behaviour expected during the melt falling stage: when the high-temperature melt enters the water pool, a vapour film forms around the melt surface and acts as a thermal resistance, strongly reducing the heat transfer between the melt and the surrounding water [1, 28]. Preliminary simulations performed with the standard mixture temperature model led to an undesired cooling of the melt during the falling stage, even when the effective thermal conductivity was set to zero, because the melt and water temperatures were averaged within the VOF interface cells. Solving two separate phase-temperature equations prevents this artificial cooling and allows the heat exchange to be activated only in the region where cooling and spreading effects are intended to be represented.

The reference temperature was chosen equal to the initial water temperature:

$$T_{ref} = T_W(t = 0) = 90^\circ\text{C} = 363\text{ K} \quad (3.21)$$

A reference volumetric sensible enthalpy was defined for the melt as [2]:

$$H_0 = \rho_M c_{p,M} (T_{M,in} - T_{ref}) \left[\frac{\text{J}}{\text{m}^3} \right] \quad (3.22)$$

where ρ_M is the melt density, $c_{p,M}$ is the melt specific heat capacity, and $T_{M,in}$ is the inlet melt temperature. Using the values adopted in the simulation:

$$H_0 = 6835 \cdot 280 \cdot (909.2 - 90) = 1.5678 \times 10^9 \left[\frac{\text{J}}{\text{m}^3} \right] \quad (3.23)$$

To represent the thermal content of each phase by means of a dimensionless passive scalar, the sensible enthalpy contribution of each phase was weighted by the corresponding VOF volume fraction and normalised with respect to the reference melt volumetric sensible enthalpy H_0 . Therefore, the melt passive scalar was defined as:

$$\phi_M = \frac{\alpha_M \rho_M c_{p,M} (T_M^* - T_{ref})}{H_0} \quad (3.24)$$

while the water passive scalar was defined as:

$$\phi_W = \frac{\alpha_W \rho_W c_{p,W} (T_W^* - T_{ref})}{H_0} \quad (3.25)$$

Here, T_M^* and T_W^* are the melt and water temperatures, reconstructed from the two transported scalars ϕ_M and ϕ_W respectively.

The reconstructed melt temperature is calculated as:

$$T_M^* = T_{ref} + \frac{H_0 \phi_M}{\rho_M c_{p,M}} \text{ [K]} \quad (3.26)$$

which, replacing the H_0 term, the equation becomes:

$$T_M^* = T_{ref} + \phi_M (T_{M,in} - T_{ref}) \text{ [K]} \quad (3.27)$$

The reconstructed water temperature is calculated as:

$$T_W^* = T_{ref} + \frac{H_0 \phi_W}{\rho_W c_{p,W}} \text{ [K]} \quad (3.28)$$

The two transported scalar fields were initialised and limited to behave as dimensionless indicators of the normalised sensible enthalpy introduced into the domain during the transient melt injection. At the beginning of the calculation, no passive scalar contribution was assigned to either phase. Therefore, both the melt and water transported scalar fields were initialised to zero throughout the computational domain:

$$\phi_M(t=0) = \phi_W(t=0) = 0 \quad (3.29)$$

This initialisation ensures that the scalar fields do not contain any artificial thermal contribution before the beginning of the melt release. The thermal scalar associated with the melt is instead introduced progressively through the nozzle inlet. At this boundary, the melt passive scalar was prescribed equal to unity, representing the reference normalised sensible enthalpy of the incoming melt, whereas the water passive scalar was set equal to zero, since no water scalar contribution is injected through the melt inlet:

$$\phi_M = 1 \quad \phi_W = 0 \quad (3.30)$$

At the pressure outlet, both transported scalars were assigned a value equal to 0:

$$\phi_M = \phi_W = 0 \quad (3.31)$$

This condition prevents any scalar contribution from being introduced into the domain in the event of local backflow through the outlet boundary. For outward flow, the scalar fields are simply convected out of the computational domain. At the solid walls, a zero-normal-flux condition was imposed, so that no passive scalar could enter or leave the domain through impermeable boundaries:

$$\nabla \phi_i \cdot \mathbf{n} = 0 \quad i = M, W \quad (3.32)$$

In the present formulation, the transported scalars were transported only by the resolved velocity field. Molecular diffusion and turbulent diffusion were therefore neglected, so that the scalar transport was used as a purely convective thermal marker. This choice was adopted to preserve the local association between the scalar value and the motion

of the corresponding phase, avoiding an artificial diffusive spreading of the normalised enthalpy field across the interface. During the transient calculation, both transported scalars were also limited within the interval $0 \leq \phi_i \leq 1$ to prevent numerical overshoots or undershoots from producing non-physical scalar values. Table 3.6 schematises the initial and boundary conditions of the transported scalar fields.

Table 3.6: Initial and boundary conditions imposed on the transported scalar fields.

Region / boundary	Melt scalar ϕ_M	Water scalar ϕ_W
Initial condition	0	0
Nozzle inlet	1	0
Pressure outlet	0	0
Solid walls	$\nabla \phi_M \cdot \mathbf{n} = 0$	$\nabla \phi_W \cdot \mathbf{n} = 0$

3.8.2. Source term and interfacial heat exchange

A source term was introduced in the phase-temperature transport equations to transfer the normalised thermal content from the melt scalar to the water scalar. This source term was not active during the entire melt fall: instead, it was activated only after the melt had penetrated below a prescribed activation depth z_{act} in the water pool.

As discussed in Section 2.5, this gating reproduces the thermal insulation provided by film boiling during the fall, while allowing the cooling to become effective only once the melt approaches the lower region of the pool and starts spreading.

The interfacial heat exchange between melt and water was modelled through a simplified conductive resistance approach. In the VOF framework, heat exchange between the two phases occurs across interfacial cells, where both melt and water are simultaneously present. Within each such cell, the unresolved thermal exchange is approximated by considering two conductive resistances in series: one associated with the melt side and one with the water side. Each resistance is estimated using Fourier's law applied over a length scale equal to the local cell size Δn , defined as the cubic root of the cell volume:

$$\Delta n = V_{\text{cell}}^{1/3}. \quad (3.33)$$

This length scale represents the characteristic dimension of the interfacial cell and provides a mesh-consistent estimate of the conduction path available within the cell for each phase. The two resistances per unit area are therefore $k_M/\Delta n$ and $k_W/\Delta n$, and their series combination gives [1]:

$$R''_{eq} = \Delta n \left(\frac{1}{k_M} + \frac{1}{k_W} \right) \left[\frac{\text{m}^2\text{K}}{\text{W}} \right], \quad (3.34)$$

It should be noted that this formulation does not imply that each phase occupies exactly half the cell. Rather, Δn is used as a single representative length scale for the entire interfacial cell, and the series combination is intended to account for the fact that heat must be conducted through both phases before being exchanged. Since in the present configuration $k_M = 5.3 \text{ W}/(\text{mK})$ and $k_W = 0.62 \text{ W}/(\text{mK})$, the water-side resistance dominates, which is physically consistent with the expectation that the liquid water side controls the thermal exchange in film-boiling-adjacent conditions.

The interfacial heat flux was then written as [1]:

$$\dot{q}''_{th} = \frac{T_M^* - T_W^*}{R''_{eq}} \left[\frac{\text{W}}{\text{m}^2} \right] \quad (3.35)$$

To obtain a volumetric heat-transfer rate, the interfacial heat flux was multiplied by the magnitude of the melt volume-fraction gradient $|\nabla\alpha_M|$. This term has a unit of $[\frac{1}{\text{m}}]$ and is non-zero only in the interfacial cells, where the phase fraction changes rapidly in space. It therefore acts as a natural localisation operator, concentrating the heat exchange at the melt–water interface [1]:

$$\dot{q}'''_{th} = \frac{(T_M^* - T_W^*) |\nabla\alpha_M|}{R''_{eq}} \left[\frac{\text{W}}{\text{m}^3} \right] \quad (3.36)$$

The volumetric heat-transfer rate is finally converted into source terms for the two phase-temperature transport equations (Eq. 3.20) by normalising it with the reference volumetric sensible enthalpy H_0 . Since $\dot{q}'''_{th}$ has units of W/m^3 and H_0 has units of J/m^3 , their ratio has units of s^{-1} , which is consistent with the source term S_{ϕ_i} of a dimensionless transported scalar. The two contributions are added with opposite signs, so that a positive heat transfer from melt to water decreases the melt scalar and increases the water scalar.

Crucially, this heat exchange is not active throughout the entire transient: it is switched on only once the melt has penetrated below the prescribed activation depth z_{act} , introduced above to reproduce the insulating effect of film boiling during the fall. This behaviour is enforced through a spatial gate based on the vertical coordinate z , so that the source terms entering the melt and water scalar equations are defined as:

$$S_{\phi_M} = \begin{cases} -\frac{\dot{q}_{th}'''}{H_0}, & z < -z_{act}, \\ 0, & z \geq -z_{act}, \end{cases} \quad S_{\phi_W} = \begin{cases} +\frac{\dot{q}_{th}'''}{H_0}, & z < -z_{act}, \\ 0, & z \geq -z_{act}, \end{cases} \quad (3.37)$$

where the z -axis points upwards with origin at the initial free surface, so that the condition $z < -z_{act}$ selects the region of the pool located below the activation depth. Above this level the source terms vanish and the melt scalar is simply convected with the flow, preserving the inlet thermal state of the falling jet; below it, the interfacial heat exchange becomes active and the melt scalar – and hence the reconstructed melt temperature T_M^* – begins to decrease. The numerical value of z_{act} was varied between the simulated cases and is reported in Chapter 4, while the corresponding STAR-CCM+ field-function implementation is given in Appendix A.

It is important to emphasise that the assumption of two conductive resistances in series within an interfacial cell is a modelling approximation, not a resolved physical description of the interfacial heat transfer. In particular, the model does not account for the actual local distribution of the two phases within the cell, does not resolve vapour film formation or condensation, and does not include convective contributions to heat transfer. Its role is to provide a numerically stable and physically motivated mechanism for transferring thermal content from the melt scalar to the water scalar in the region below the prescribed activation depth.

3.9. Melt rheology and Ramacciotti viscosity model

The viscosity of the melt is modified as a function of its local temperature to reproduce the progressive resistance to spreading associated with cooling and partial solidification. The equivalent solid fraction is obtained directly from the reconstructed melt temperature T_M^* , rather than from a resolved enthalpy balance.

The solidus and liquidus temperatures adopted for the melt material are reported in Table 3.7.

Table 3.7: Solidus and liquidus temperatures adopted for the melt material [11].

Temperature	Value [K]	Value [°C]
Solidus temperature, T_{sol}	1143	870
Liquidus temperature, T_{liq}	1189	916

Although the nominal eutectic composition reported for the reference material is associ-

ated with a melting temperature of 870°C , the liquidus temperature used in the simulation was increased to account for the alteration of the melt composition caused by the interaction between the melt and the crucible material during preparation. The numerical solidification interval was therefore defined between 870°C and 916°C [11].

A normalised temperature was introduced as [22]:

$$T^* = \frac{T_M^* - T_{sol}}{T_{liq} - T_{sol}}. \quad (3.38)$$

The equivalent solid fraction was then calculated as [22]:

$$f_s = \begin{cases} 1, & T^* \leq 0, \\ 1 - T^*, & 0 < T^* < 1, \\ 0, & T^* \geq 1. \end{cases} \quad (3.39)$$

The apparent viscosity of the melt was evaluated using the Ramacciotti-type exponential law [21]:

$$\mu_M = \mu_0 \exp(2.5Cf_s), \quad (3.40)$$

where:

- μ_0 is the viscosity of the fully liquid melt;
- C is an empirical coefficient
- f_s is the equivalent solid fraction.

The coefficient C controls the intensity of the viscosity increase during cooling. Higher values of C lead to a stronger increase in viscosity and therefore to a faster deceleration of the melt front. Lower values of C keep the melt more mobile for a longer time and favour larger spreading distances. In this work, different values of C were tested as part of a sensitivity analysis.

3.10. Model assumptions and limitations

The numerical model developed in this work is based on several simplifying assumptions.

1. The melt-coolant system is modelled with only two phases, the molten material

and liquid water. In the real experiment, however, the interaction is intrinsically a three-phase process, because a large amount of water vapour is generated at the melt surface, both through film boiling during the fall and through the intense boiling that accompanies the spreading on the plate. In the present model the vapour is not represented as a separate fluid: its insulating thermal effect during the fall is reproduced only indirectly, through the activation-depth mechanism, while its dynamic effects — such as the reduced drag on the melt and the agitation of the pool — are neglected. A fully consistent description would require a three-phase formulation (melt, liquid water and vapour), which is beyond the scope of the present work.

2. The thermal field is described by two phase-temperature transport equations rather than by a complete multiphase energy balance. The melt–water heat exchange is represented through a simplified, depth-activated source term, and the vapour phase is neglected. The reconstructed melt and water temperatures are therefore affected by these simplifications, especially during the falling stage, where the insulating effect of film boiling is reproduced only in an approximate way.
3. Film boiling is not directly modelled through a dedicated boiling or phase-change model. Its effect is represented indirectly by suppressing heat exchange during the falling stage and activating the heat-exchange source term only below a prescribed depth. This approach allows the numerical model to avoid artificial cooling of the melt during fall, but it does not resolve vapour film dynamics, bubble formation, condensation, or water evaporation.
4. The solidification process is not obtained from a resolved enthalpy balance. The equivalent solid fraction is obtained from the melt temperature and is used only to modify the melt viscosity through the Ramacciotti model.
5. The numerical model does not explicitly reproduce melt fragmentation, porous debris formation, crust rupture, or detailed steam escape channels. These phenomena are relevant in the real experiment, where the final debris bed may contain fragmented material, solidified cake regions, porosity, and eruptive structures, as described in the experimental results. These mechanisms require the explicit resolution, or modelling, of melt breakup, phase change, vapour production, debris-scale porosity, and mechanical crust failure. In the present CFD formulation, the VOF model represents the melt and water as continuous phases separated by a resolved interface, while solidification effects are introduced indirectly through the temperature-based viscosity model.

Despite these limitations, the model provides a useful framework for analysing the main hydrodynamic spreading behaviour of the melt.

4 | Numerical Results and Discussion

This chapter presents the results obtained from the different simulation cases developed during the modelling process of the PULiMS-E10 experiment. The objective is not only to present the final numerical configuration, but also to clarify the role of each modelling choice and the reason why the model was progressively modified.

4.1. Introduction and overview of the simulated cases

The simulations are organised as a sequence of cases with increasing modelling complexity:

- Case 1 represents the starting point of the analysis and is used to investigate the behaviour of the directly solved temperature field when the thermal conductivity of the melt, water, and mixture is set to an almost negligible value. The results of the case motivated the development of a more controlled thermal treatment based on transported scalars.
- Case 2 represents the two-temperature thermal model introduced in Chapter 3 and in this configuration, transported scalars are used to control the thermal interaction for both melt and water. The purpose of this case is to show that the melt temperature remains unchanged during the initial falling stage of the jet and starts to evolve only after the prescribed activation depth is reached. However, the viscosity is still kept constant meaning that the model cannot represent a progressive loss of melt mobility. Therefore, Case 2 is mainly used to demonstrate the functioning of the two-temperature thermal formulation, rather than to reproduce the final spreading behaviour.
- Cases 3A and 3B include the coupling between the two-temperature thermal model and the Ramacciotti viscosity formulation. Both cases use the same activation depth while the Ramacciotti coefficient is varied. These simulations are used to evaluate the effect of the viscosity-growth coefficient on melt mobility and spreading.

Although the introduction of the Ramacciotti model allows the melt viscosity to increase as the phase-temperature field evolves, the simulations still show limitations in reproducing the accumulation observed in the experimental impact region.

- For this reason, Cases 4A and 4B introduce a modified thermal treatment in the impact region. The activation depth is increased and the volumetric heat flux is multiplied by a factor A inside a prescribed impact-region control volume. The purpose of this modification is to enhance the local heat extraction in the impact region and to promote a more pronounced melt immobilisation close to the initial contact area, as suggested by the experimental evidence. As for Cases 3A and 3B, Case 4A differs from Case 4B in the value of the Ramacciotti coefficient C , allowing the combined effect of the enhanced heat extraction and of the viscosity-growth coefficient to be analysed.

Table 4.1: Summary of the main modelling parameters adopted in the numerical cases analysed in Chapter 4.

Case	Thermal conductivity [W/(m K)]	Two-temperature thermal model	Ramacciotti model	C	Source-term activation depth [m]	A
Case 1	10^{-10}	OFF	OFF	–	–	OFF
Case 2	M: 5.3; W: 0.62	ON	OFF	–	0.1212	OFF
Case 3A	M: 5.3; W: 0.62	ON	ON	4	0.1212	OFF
Case 3B	M: 5.3; W: 0.62	ON	ON	2	0.1212	OFF
Case 4A	M: 5.3; W: 0.62	ON	ON	4	0.16	1000
Case 4B	M: 5.3; W: 0.62	ON	ON	2	0.16	1000

Note: M and W denote the melt and water phases, respectively.

All the cases listed in Table 4.1 were run with the same mesh, adaptive mesh refinement and time-step settings described in Chapter 3; in particular, they share the same adaptive time step, which rapidly reaches its lower bound of 2×10^{-4} s. For this reason the time step is not repeated in the table, and the cases differ only in the modelling parameters reported there.

The discussion of the results follows the same order reported in Table 4.1. Each case is analysed with respect to the specific modelling issue it was designed to address. The comparison with the experimental behaviour is progressively introduced when relevant, with particular attention to the spreading dynamics, accumulation in the impact region, and final melt distribution.

4.2. Preliminary verification of the thermal treatment on a 2D test case

Before applying the model to the full PULiMS-E10 geometry, the thermal treatment was examined on a simplified two-dimensional test case, designed to isolate the behaviour of the temperature field from the complexity of the falling jet and of the spreading dynamics. The computational domain is a square two-dimensional cell – a vertical slice in which the out-of-plane direction is treated as effectively infinite – initially filled with melt (M) in one half, at the inlet temperature $T_{M,in} = 1182.2$ K, and with water (W) in the other half, at $T_W = 363$ K, the two phases being separated by a sharp interface. All the configurations were run as transient (implicit unsteady) simulations, consistently with the full model. This controlled configuration makes it possible to address three distinct questions in sequence: how the temperature obtained from a single energy equation behaves under pure conduction, what is the numerical origin of the spurious cooling that can affect a directly solved temperature field across the melt–water interface, and whether the two-temperature formulation reproduces the intended thermal behaviour. The four configurations analysed on this test case are summarised in Table 4.2.

In all cases the two phases are initialised at rest and each fills one half of the cell at its own uniform temperature, with the melt volume fraction set to one in the melt half and to zero in the water half (and vice versa for the water), so that the planar melt–water interface is initially sharp. Since the simulations are transient, the conduction case shows the developing thermal boundary layer rather than the asymptotic uniform temperature that pure conduction would eventually produce if run to steady state. The time step used in each configuration is reported in Table 4.2: the at-rest conduction cases are essentially insensitive to it, whereas its role is precisely what the third configuration is designed to investigate.

Table 4.2: Configurations analysed on the 2D test case.

Configuration	Thermal conductivity k [W/(m K)]	Gravity	Thermal treatment	Time step Δt [s]
Conduction, $k \neq 0$	M: 5.3; W: 0.62	OFF	energy equation	not critical (at rest)
Conduction, $k = 0$	0	OFF	energy equation	not critical (at rest)
Time-step sensitivity	0	ON	energy equation	0.1 vs 0.001
Two-temperature model	M: 5.3; W: 0.62	ON	two-temperature model	0.001

Note: M and W denote the melt and water phases, respectively.

4.2.1. Conduction with and without thermal conductivity

In the first configuration the fluids are kept at rest ($\mathbf{u} = 0$): gravity is switched off so that the interface stays stationary and the temperature field can evolve only by conduction. Conduction is, in fact, the only mechanism of heat exchange between the two immiscible phases regardless of gravity; removing gravity simply suppresses any buoyancy-driven motion and isolates the conductive behaviour from advective transport. When a finite thermal conductivity is assigned to the two phases, a thermal boundary layer develops at the melt–water interface: the melt is locally cooled and the water is locally heated, while the bulk of each phase, far from the interface, remains close to its initial temperature, since the simulation is transient and still far from the steady state at which conduction would eventually make the temperature uniform (Figure 4.1a). When the thermal conductivity is instead set to zero, the temperature field does not evolve at all and the two phases retain their initial temperatures, with a perfectly sharp interface (Figure 4.1b).

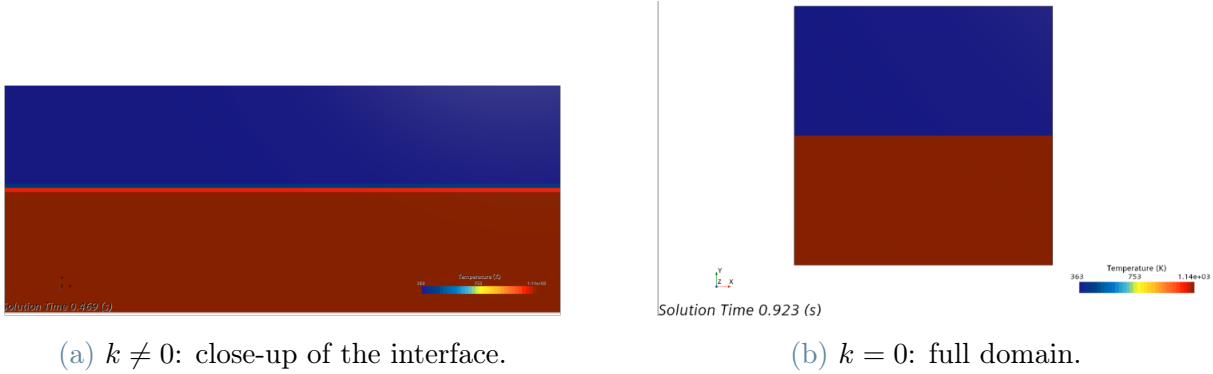


Figure 4.1: Temperature field in the quiescent 2D test ($\mathbf{u} = 0$, no gravity): (a) with finite thermal conductivity a thermal exchange layer develops at the interface (the melt cools and the water heats locally); (b) with $k = 0$ the two phases retain their initial temperatures and the interface stays sharp.

This first test confirms the expected behaviour of the directly solved temperature in a quiescent system: heat is exchanged only through conduction, and no exchange occurs when the conductivity is suppressed. It therefore establishes a baseline against which the next configuration can be interpreted.

4.2.2. Interface-transport error and time-step sensitivity

In the second configuration gravity is activated while the thermal conductivity is kept at zero. The melt and water are initialised as in the previous configuration, each filling one half of the cell – the melt at $T_{M,in} = 1182.2$ K and the water at $T_W = 363$ K – but now

placed side by side in the gravity field. Because the denser melt and the lighter water are arranged in this way, the configuration is gravitationally unstable and a buoyancy-driven motion sets in, advecting and folding the interface. Since the conductivity is zero, no physical heat exchange between the phases is possible: any change in the temperature field is therefore of purely numerical origin, arising from the averaging of the two phase temperatures within the interfacial (mixture) cells and from the numerical diffusion associated with the advection of the temperature across a non-sharp interface.

Figure 4.2 compares the temperature field at the same physical time ($t = 0.3$ s) for two different time steps. With a coarse time step ($\Delta t = 0.1$ s) the interface is strongly smeared and the temperature field is heavily diffused, so that large regions of intermediate, unphysical temperature appear even though the conductivity is zero (Figure 4.2a). With a much finer time step ($\Delta t = 0.001$ s) the interface remains sharp, the buoyancy-driven roll-ups are well resolved, and the spurious temperature diffusion is markedly reduced (Figure 4.2b).

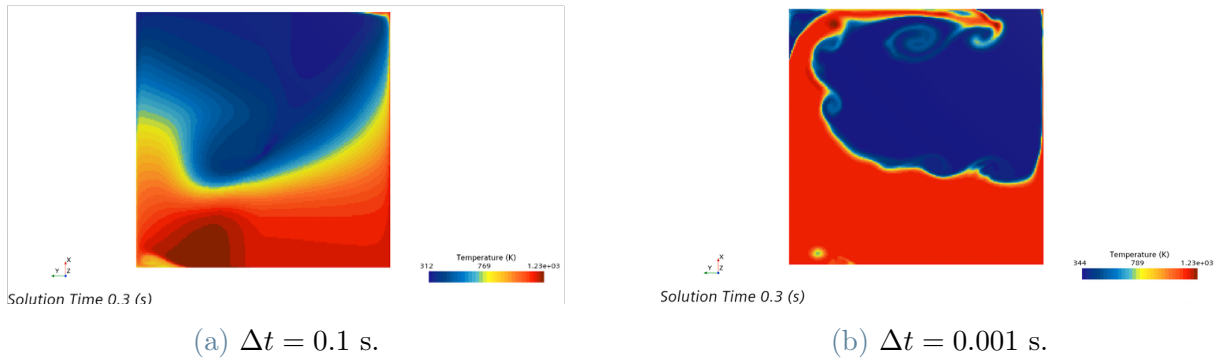


Figure 4.2: Temperature field in the 2D test with gravity active and $k = 0$, at $t = 0.3$ s, for two time steps: (a) a coarse time step produces a strongly smeared interface and a diffused temperature field (large interface-transport error); (b) a fine time step preserves a sharp interface and a well-resolved temperature field.

This test isolates the numerical origin of the artefact that will later be observed in Case 1 (Section 4.3), where the melt appears to cool during the fall even with a near-zero conductivity. The apparent cooling does not stem from a resolved conductive process but from the interface-cell averaging of the two phase temperatures, an error that grows as the interface becomes less sharp. It is worth stressing that the test case is run with a laminar model, so that no turbulent transport and, in particular, no turbulent Prandtl number are involved: the only physical mechanism able to redistribute heat would be molecular conduction (here suppressed by setting $k = 0$), so the residual temperature changes are purely numerical and governed by the time step. Because a sufficiently fine interface res-

olution cannot be guaranteed everywhere and at all times in the full transient simulation, the directly solved temperature is not a reliable control variable for the cooling-induced rheology, which motivates the two-temperature treatment adopted in this work.

4.2.3. Two-temperature thermal model

The same configuration was finally simulated with the two-temperature thermal model described in Chapter 3. As shown in Figure 4.3a, in the early instants the reconstructed melt temperature T_M^* is uniform and exactly equal to the inlet value of 1182.2 K throughout the melt: the bulk thermal state is preserved and no spurious cooling is introduced. As the interface deforms under gravity (Figure 4.3b), the thermal exchange remains confined to the interfacial cells, where T_M^* varies only within a narrow range close to the initial value, while the melt bulk remains at 1182.2 K.

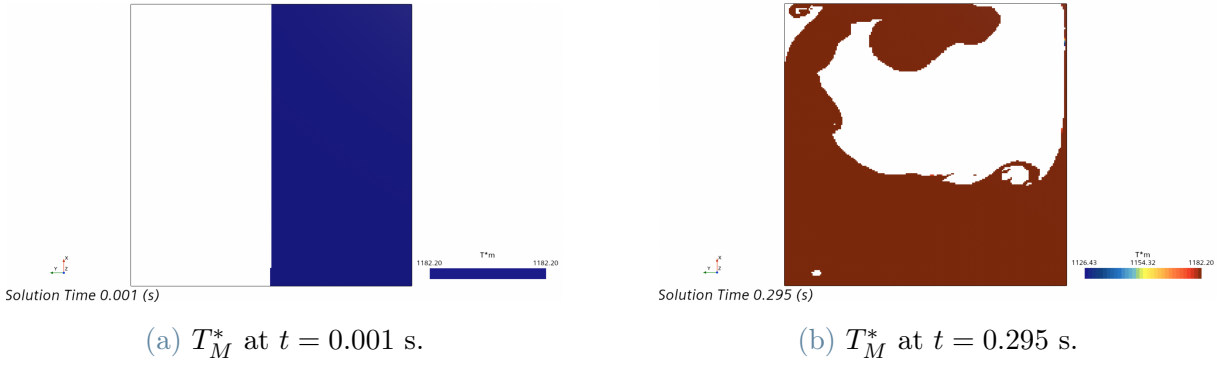


Figure 4.3: Reconstructed melt temperature T_M^* in the 2D test with the two-temperature thermal model: (a) the melt bulk remains uniformly at the inlet temperature of 1182.2 K; (b) once the interface deforms, the thermal exchange is confined to the interfacial cells (note the narrow colour scale), without affecting the melt bulk.

This last test confirms that the two-temperature formulation reproduces the intended behaviour: contrary to the directly solved temperature, it does not introduce any spurious cooling of the melt bulk, while still allowing a controlled thermal exchange that is correctly localised at the melt–water interface. This result provides the justification, on a controlled configuration, for the modelling strategy adopted in the full PULiMS-E10 simulations discussed in the remainder of this chapter.

4.3. Case 1: Direct temperature solution with negligible thermal conductivity

Case 1 was performed to assess the behaviour of the directly solved temperature field during the initial interaction between the melt and the water pool. In this simulation, the thermal conductivity of the melt, water, and mixture was set equal to $k = 10^{-10} [W/(mK)]$, so that conductive heat transfer was practically suppressed. No two-temperature thermal model was used, and the Ramacciotti viscosity formulation was not active. The initial melt temperature was 1182.2 K, while the initial water temperature was 363 K. These values are the reference initial temperatures adopted throughout the numerical campaign.

The purpose of this case was not to reproduce the experimental spreading behaviour, but to verify whether the direct temperature solution could be used as a reliable control variable for the subsequent modelling of melt cooling and immobilisation. In principle, if the thermal conductivity is set to an almost negligible value, the temperature field should not evolve significantly due to conduction. Therefore, any relevant variation of the melt temperature during the first stages of the simulation would indicate that the directly solved temperature field is affected by mechanisms other than pure conductive heat transfer.

This test is particularly important because the temperature field would directly influence the melt dynamics if it were coupled with a temperature-dependent viscosity or with a solid-fraction-dependent immobilisation model. In that case, an artificial or uncontrolled decrease of temperature during the falling stage would lead to a premature increase in solid volume fraction and, consequently, to an unrealistic modification of the melt motion before the jet reaches the region where heat exchange is intended to become relevant.

4.3.1. Temperature and solid-fraction evolution with negligible thermal conductivity

The simulation was advanced up to approximately $t=0.31$ s. The first instants of melt entry into the pool were analysed using contours extracted on the symmetry plane. Figure 4.4 shows the temperature field during the early phase of the transient. Although the melt is initially injected at 1182.2 K and the thermal conductivity is set to an almost null value, the contour sequence shows that the temperature field is not preserved during the melt fall and early interaction with water.

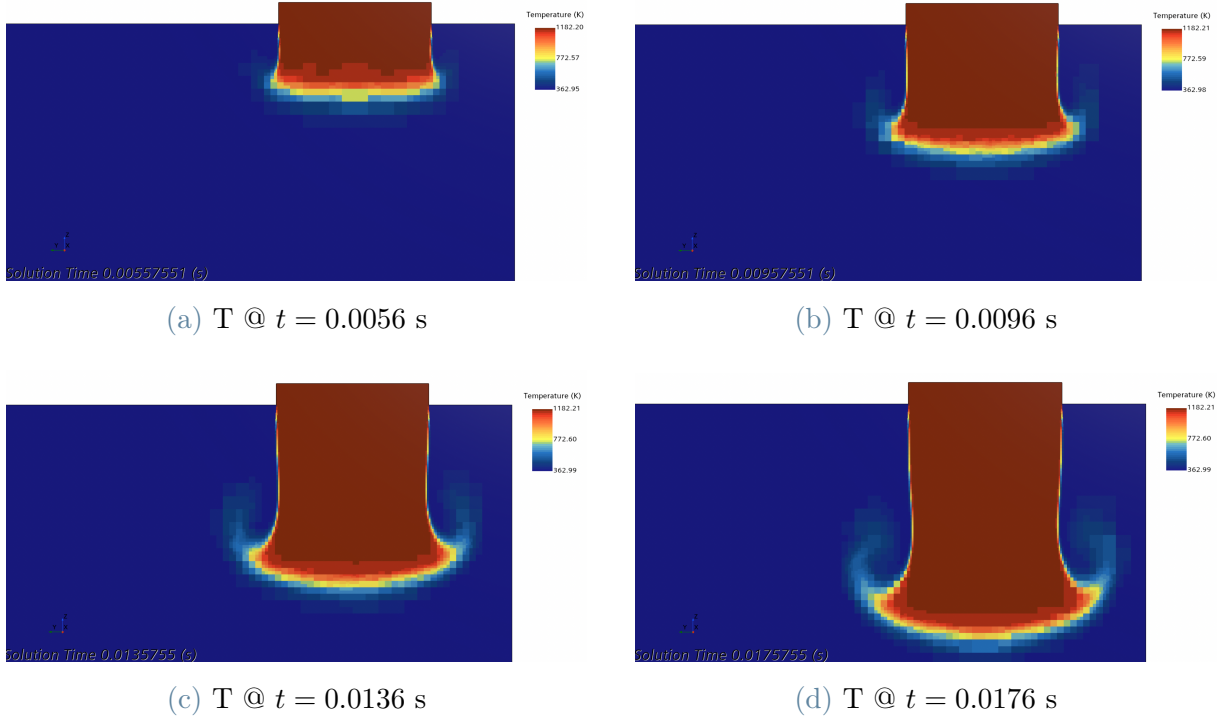


Figure 4.4: Melt temperature countours in the early stages of melt entry into the water pool on the symmetry wall for Case 1.

The decrease is visible close to the melt-water interface and progressively affects the region surrounding the lower part of the jet. The temperature contours show the development of a colder layer around the melt, together with local temperature variations near the lateral interface. This behaviour is not consistent with the intended use of the direct temperature field as a controlled indicator of thermal exchange, because the temperature starts to evolve before the introduction of the two-temperature thermal treatment and before any phenomenological viscosity model is activated.

The same behaviour is reflected in the solid volume fraction field. Figure 4.5 shows that the solid volume fraction of the melt increases during the early transient. This increase is observed not only at the external interface, but also within regions of the melt bulk. As a consequence, if the flow model were coupled directly to a viscosity or immobilisation law based on temperature or solid fraction, the melt dynamics would be affected from the beginning of the simulation. This would introduce an undesired solidification effect during the falling and early impact stages.

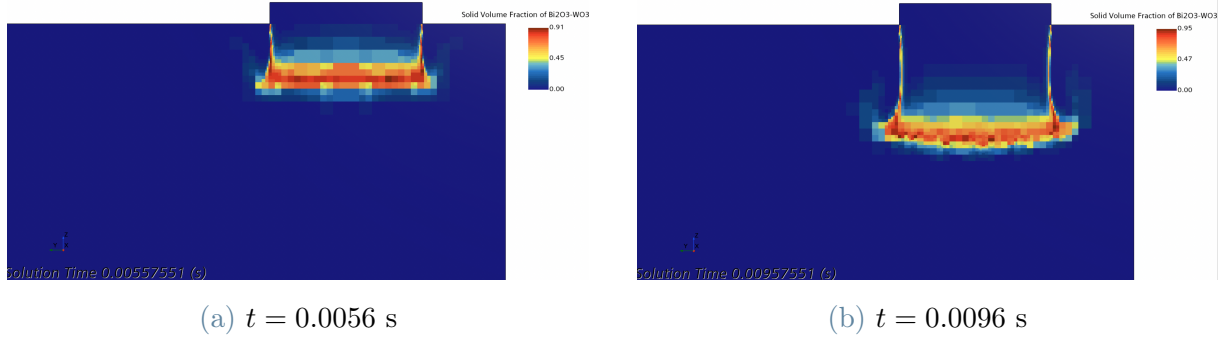


Figure 4.5: Solid volume fraction contours on the symmetry wall for Case 1 during the early melt entry into the water pool.

The combination of the temperature and solid volume fraction fields indicates that the direct solution of the temperature equation is not suitable for the modelling strategy adopted in this work. The main point is that, under the imposed condition of negligible thermal conductivity, the temperature and solid fraction still evolve during the initial motion of the jet. This suggests that the computed thermal field is influenced by the multiphase transport of temperature, interface motion, and the numerical treatment of mixed cells in the VOF framework.

4.4. Case 2: Two-temperature thermal model with constant viscosity

Case 2 introduces the two-temperature thermal model described in Chapter 3. It is, in effect, Case 1 re-run with the new thermal treatment: the geometry, the mesh and the operating conditions are identical, the only difference being that the melt thermal state is no longer governed by a single, directly solved temperature field. The simulation was carried out up to approximately $t = 0.23$ s. Instead of the directly solved temperature, the flow solver is run in isothermal mode and a melt temperature T_m^* is reconstructed through field functions from the two-temperature formulation, and is used to control the thermal state of the melt.

The objective of this case is to verify whether the developed two-temperature model is able to preserve the initial melt temperature during the falling stage and to activate the thermal exchange only after a prescribed penetration depth. The activation depth is set equal to 0.1212 m, corresponding to a height of 0.0788 m above the bottom of the pool. The melt viscosity is kept constant and equal to 0.016 Pa s; therefore, this case does not include any viscosity increase or immobilisation effect.

4.4.1. Activation and temperature evolution

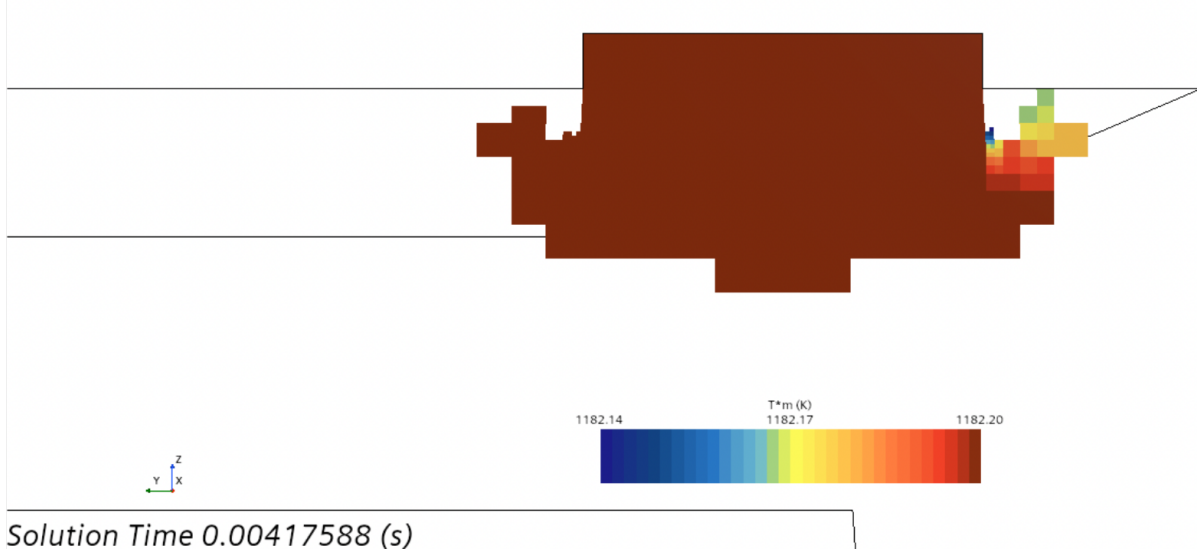


Figure 4.6: Contours of the reconstructed melt temperature T_m^* during the initial falling stage of Case 2.

The contours of the reconstructed melt temperature during the initial falling stage are shown in Figure 4.6. The first instants of the simulation show that T_m^* remains equal to the initial melt temperature during the free-fall stage. In the early frames, before the activation depth is reached, the melt is still represented at approximately 1182.2 K. This indicates that the two-temperature formulation prevents the premature temperature decrease observed in Case 1.

It should be noted that the contours in Figure 4.6, and the analogous temperature contours shown for the other cases, display the reconstructed melt temperature T_m^* , that is, the melt-phase temperature in the region where the melt is present. A single temperature field defined over the whole domain is deliberately not shown: since the model carries two separate phase temperatures (T_m^* for the melt and T_w^* for the water), a combined field would, in the interfacial cells, only reflect the volume-fraction averaging of the two phase temperatures rather than a physical temperature. For this reason only the melt-phase field, which is the quantity of interest for the cooling-induced rheology, is reported.

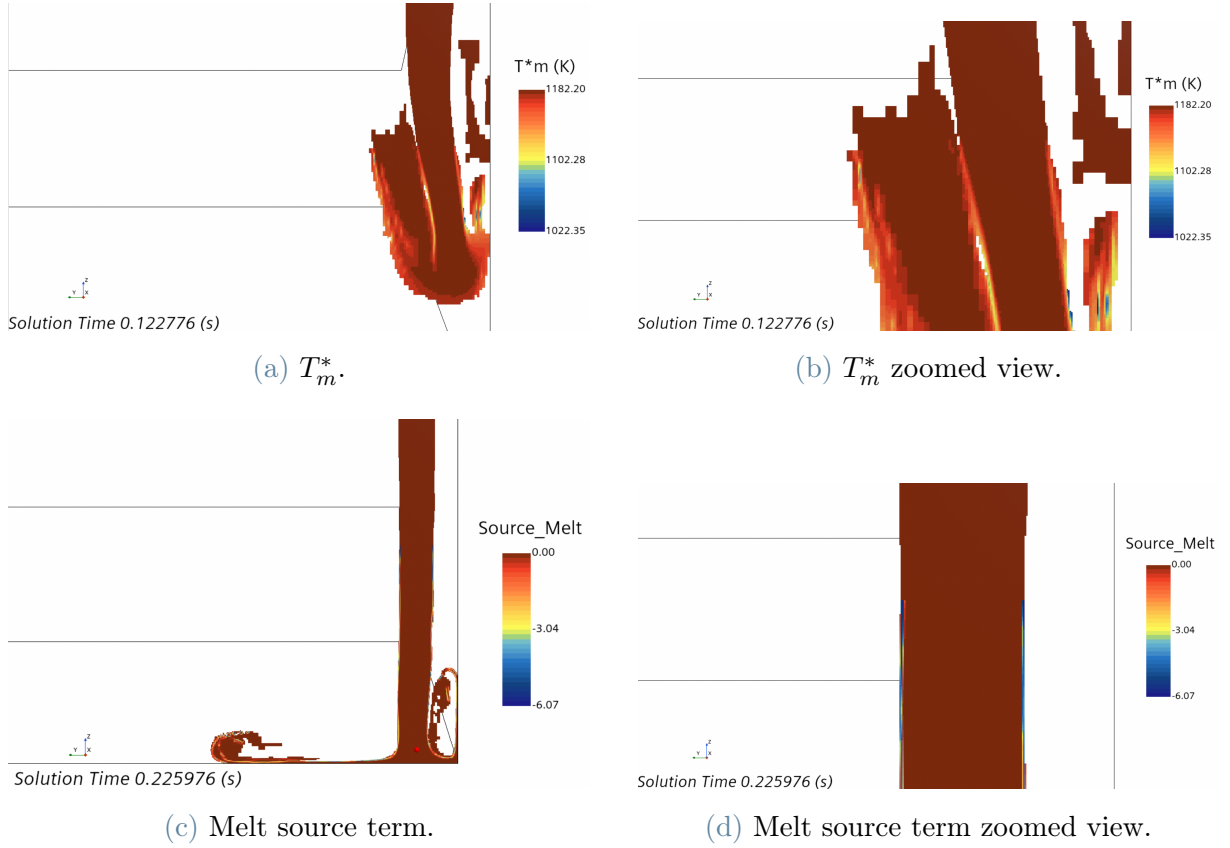


Figure 4.7: Activation of the two-temperature thermal model in Case 2. The upper panels show the reconstructed melt temperature T_m^* as the melt crosses the prescribed activation depth of 0.1212 m. The lower panels show the corresponding activation of the melt source term after the same depth threshold is reached.

The activation of the two-temperature thermal model is illustrated in Figure 4.7. Once the melt crosses the prescribed activation level, the source terms associated with the melt and water scalar fields become active. From this point, the reconstructed temperature begins to decrease in the region where the melt interacts with the water. The contours at later times show the formation of colder zones around the spreading melt, while the portion of the incoming jet above the activation level remains at the initial temperature.

This result confirms the main purpose of the two-temperature thermal model: the thermal exchange is not triggered immediately at the inlet or during the initial fall, but only after the melt reaches the selected depth. Compared with the direct temperature solution of Case 1, the two-temperature approach provides a more controlled definition of the onset of cooling.

4.4.2. Solid fraction and constant-viscosity limitation

The effect of the two-temperature thermal model is also visible in the solid volume fraction field, reported together with the reconstructed melt temperature in Figure 4.8. After activation, the solid fraction starts to increase in the cooled regions of the melt. However, in Case 2 this information is not coupled to the melt viscosity, which remains fixed at 0.016 Pa s throughout the simulation.

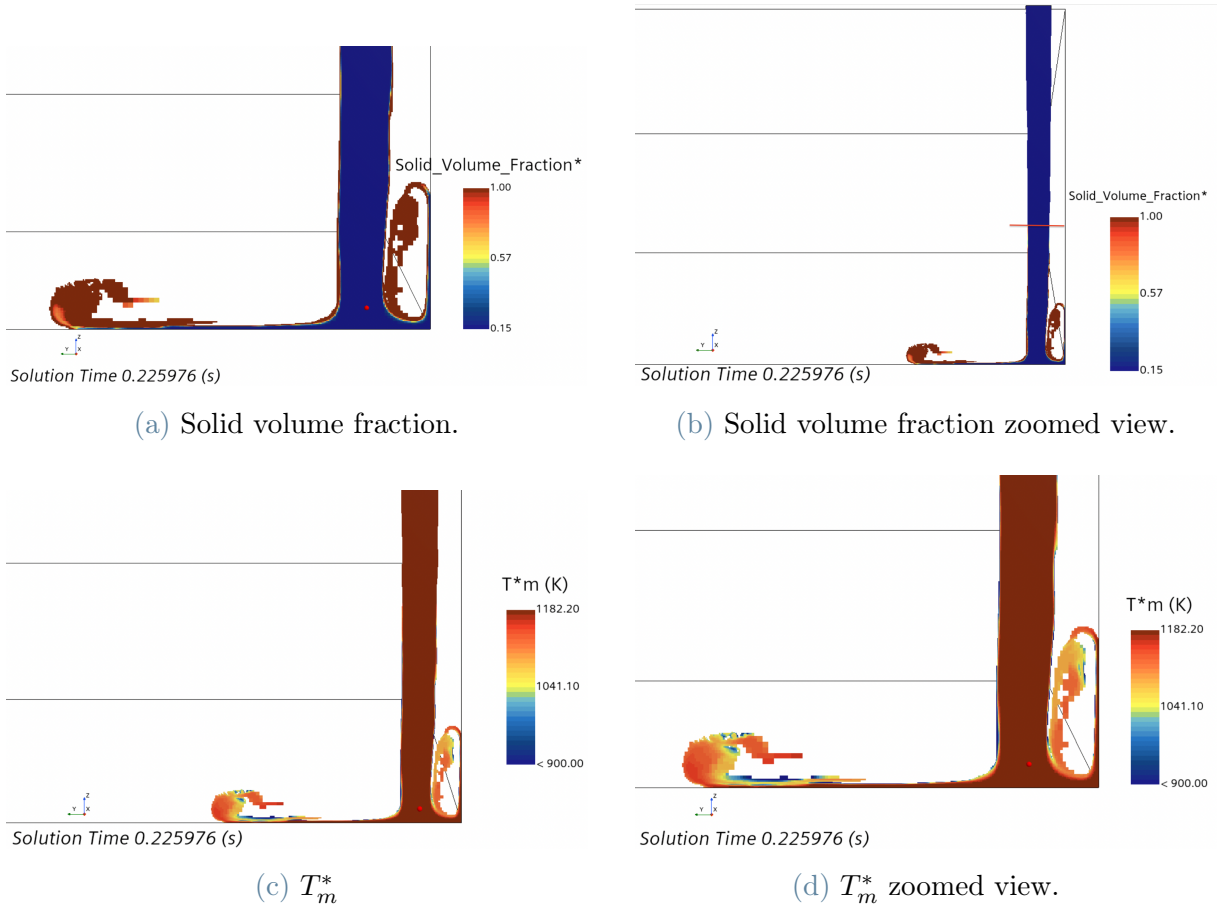


Figure 4.8: Solid volume fraction and reconstructed melt temperature at $t = 0.226$ s after jet melt impact with bottom pool for Case 2.

As a consequence, although the model reproduces the delayed onset of cooling, it cannot represent the progressive loss of melt mobility: with a constant viscosity, the cooling computed by the thermal model does not translate into any immobilisation of the melt, and no localised accumulation builds up at the impact point. For this reason, Case 2 is not intended as a predictive simulation of the final melt distribution; its role is to validate the behaviour of the two-temperature thermal formulation before coupling it with a viscosity-growth model.

4.4.3. Melt front and impact-zone temperature

The melt front position in the X - and Y -directions and the temperature monitored at the central impact-zone thermocouple are reported in Figures 4.9 and 4.10, respectively. Throughout the chapter, the numerical melt front is compared with the experimental reconstruction, and the reconstructed melt temperature T_M^* at the impact point with the experimental thermocouple TC0; it should be kept in mind that T_M^* is a reconstructed temperature (Chapter 3) and that the simulated time window is much shorter than the experimental one, so the comparison is mostly meaningful in terms of melt arrival time and qualitative trends.

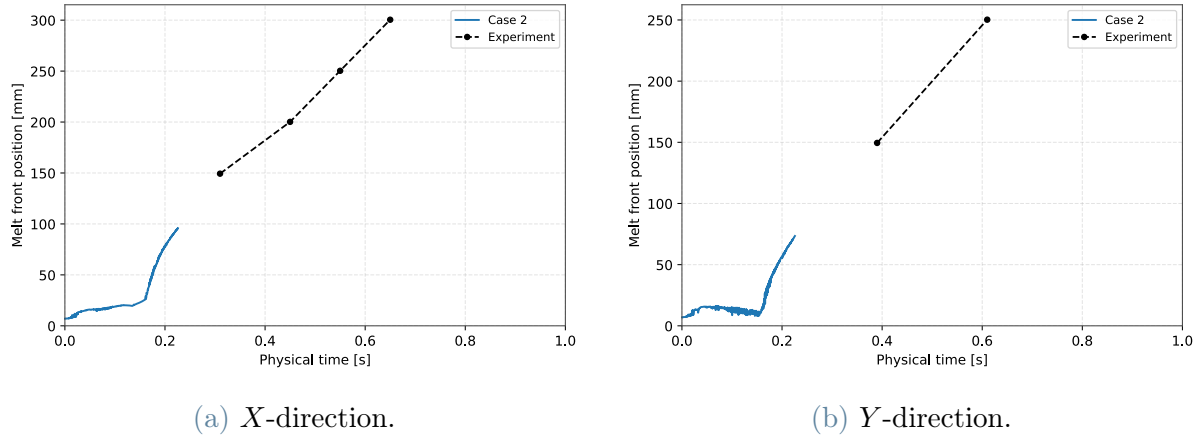


Figure 4.9: Case 2: melt front position in the X - and Y -directions, compared with the experimental reconstruction. Experimental data from [14].

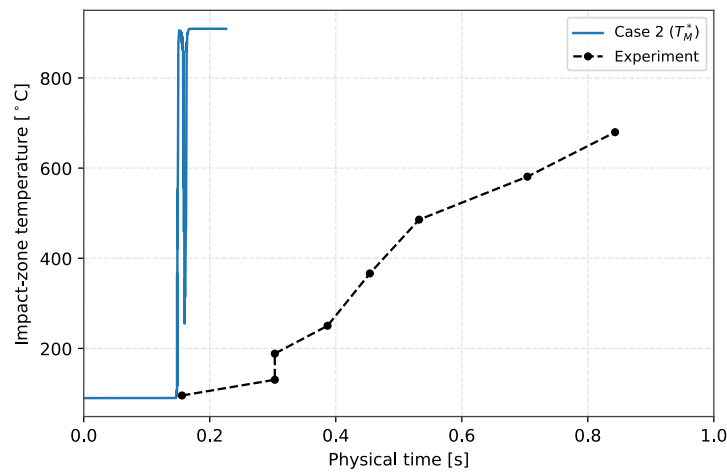


Figure 4.10: Case 2: reconstructed melt temperature T_M^* at the impact-zone thermocouple, compared with the experimental TC0 reading. Experimental data from [14].

Consistently with the constant-viscosity assumption, the melt front advances rapidly in

both directions and the melt remains highly mobile: within the short simulated window the front already reaches several centimetres. Since the viscosity is not yet allowed to increase, this stage cannot reproduce the later slowing-down and accumulation observed in the experiment, and the comparison with the measured front is only indicative at this point. The impact-zone temperature confirms that the jet reaches the centre of the plate at $t \approx 0.15$ s, in good agreement with the onset of the experimental TC0 signal (about 0.16 s); afterwards T_M^* remains close to the melt temperature, since in the absence of a viscosity increase the hot melt is not immobilised and keeps feeding the impact region.

Case 3 then introduces the Ramacciotti viscosity formulation, using the phase-temperature field as the controlling variable for the viscosity increase.

4.5. Case 3: Coupling with the Ramacciotti viscosity model

Case 3 introduces the coupling between the two-temperature thermal model and the Ramacciotti viscosity formulation [21]. The activation depth is kept equal to 0.1212 m, as in Case 2, while the melt viscosity is no longer constant. Instead, the phase-temperature field is used to increase the dynamic viscosity as the melt progressively cools down and the solid volume fraction increases.

Two values of the Ramacciotti coefficient are compared. Case 3A uses $C = 4$, while Case 3B uses $C = 2$. The objective is to evaluate how the intensity of the viscosity increase affects melt spreading, local accumulation, and mobility after impact.

4.5.1. Selection of the Ramacciotti coefficient

Before comparing the two simulations, the influence of the Ramacciotti coefficient was analysed by plotting the viscosity law as a function of the solid volume fraction, as shown in Figure 4.11. The coefficient C controls the steepness of the viscosity increase. Larger values produce a much faster growth of viscosity as the solid fraction approaches one, whereas lower values preserve a more mobile melt for the same thermal state.

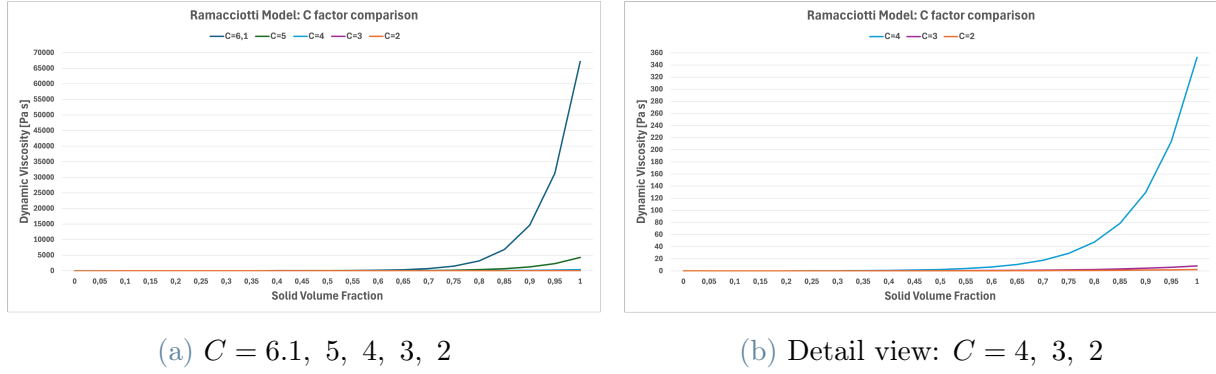


Figure 4.11: Comparison of the Ramacciotti viscosity model for different values of the coefficient C .

The value $C = 6.1$, reported in the reference formulation for the specific material considered by Ramacciotti, was not retained for the simulations discussed in this chapter. A preliminary test showed that this value produced an excessively steep viscosity increase in the present modelling framework, leading to a nearly complete immobilisation of the jet and preventing a realistic degree of melt mobility. For this reason, the discussion focuses on $C = 4$ and $C = 2$, which provide two less restrictive configurations and allow the effect of the viscosity-growth rate to be evaluated. It is worth noting that the value $C = 4$ is also adopted in the literature for an analogous problem: in the numerical study of underwater melt spreading by Zhao et al. [28], the empirical constant C_r of the Ramacciotti model is likewise set to 4 as the best-fit value resulting from their sensitivity analysis. This independent choice provides further support for the value retained as the reference case in the present work.

4.5.2. Case 3A: Reference Ramacciotti coefficient $C = 4$

Case 3A was advanced up to approximately $t = 0.91$ s. With $C = 4$, the viscosity increase becomes sufficiently strong to modify the melt motion after the onset of cooling. The temperature contour in Figure 4.12 shows that the melt remains hot in the incoming jet, while the material already spread inside the pool undergoes cooling and local solidification.

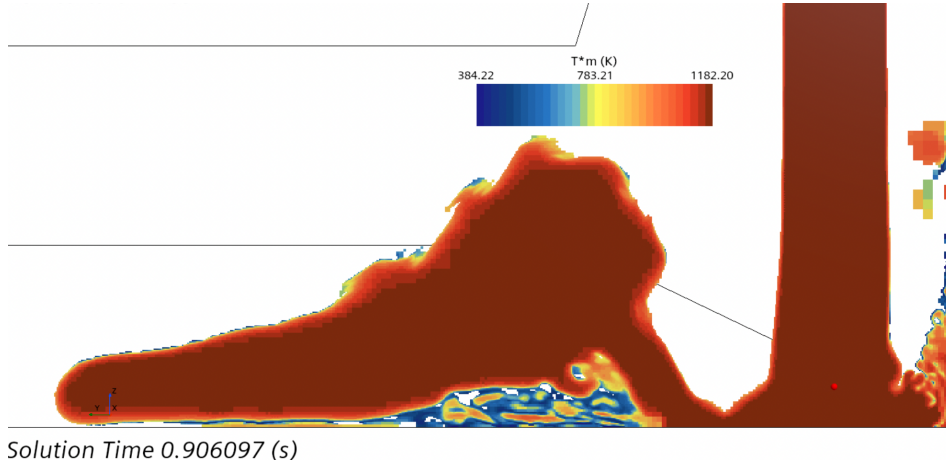


Figure 4.12: Temperature contour for Case 3A.

The corresponding solid volume fraction field (Figure 4.13) shows that the melt does not remain uniformly liquid after impact. Regions with high solid fraction develop within the deposited material, especially along the lower part of the spreading layer and around the external boundaries of the accumulation zone.

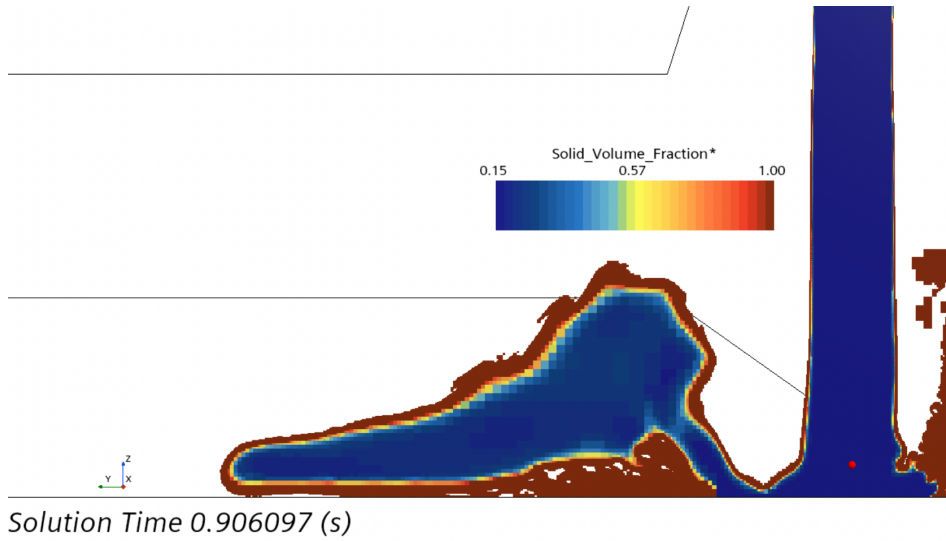


Figure 4.13: Solid volume fraction contour for Case 3A.

The viscosity field (Figure 4.14) confirms the effect of the Ramacciotti coupling. The increase in viscosity is localised in the cooled and partially solidified portions of the melt, while the incoming jet remains comparatively more mobile. As a consequence, the spreading is reduced with respect to a constant-viscosity formulation. However, the melt does not accumulate immediately in the impact region. Instead, it tends to form a depression close to the impact zone and a higher accumulation around it. This behaviour

differs from the experimental observation, where the melt starts to solidify shortly after impact and hotter material subsequently flows over the deposited layer [14].

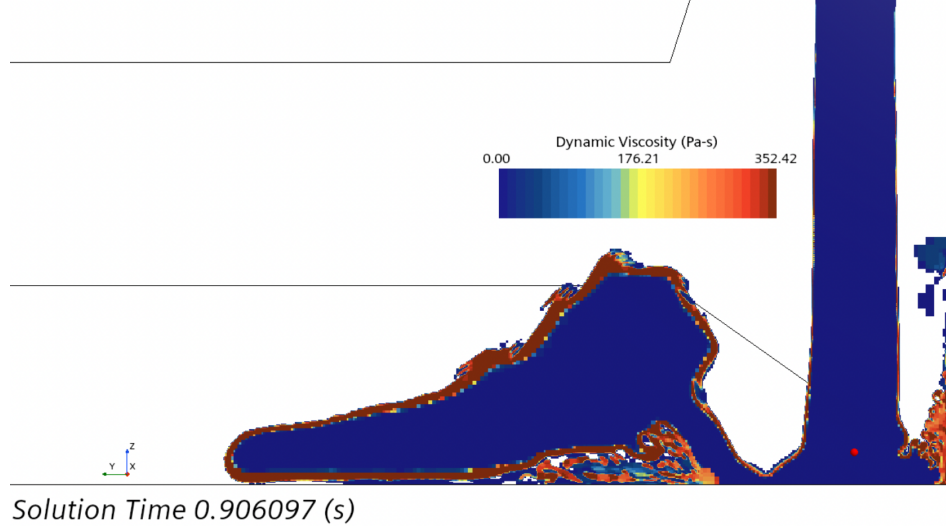


Figure 4.14: Dynamic viscosity contour for Case 3A.

4.5.3. Case 3B: Reduced Ramacciotti coefficient $C = 2$

Case 3B was simulated up to approximately $t = 0.44$ s. Reducing the coefficient to $C = 2$ makes the viscosity growth significantly weaker. The temperature field (Figure 4.15) still evolves according to the two-temperature thermal model, but the corresponding viscosity increase is not sufficient to produce a marked immobilisation of the melt.

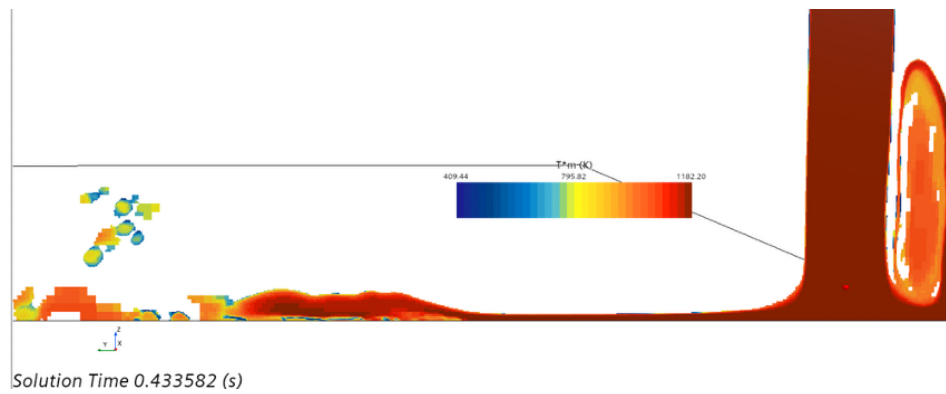


Figure 4.15: Temperature contour for Case 3B.

The dynamic viscosity (Figure 4.16) remains much lower than in Case 3A at the corresponding stages of the transient. As a result, the melt continues to behave as a highly mobile liquid layer. The contours show a thin spreading region rather than a stable accumulation zone. No clear build-up of material is obtained near the impact area.

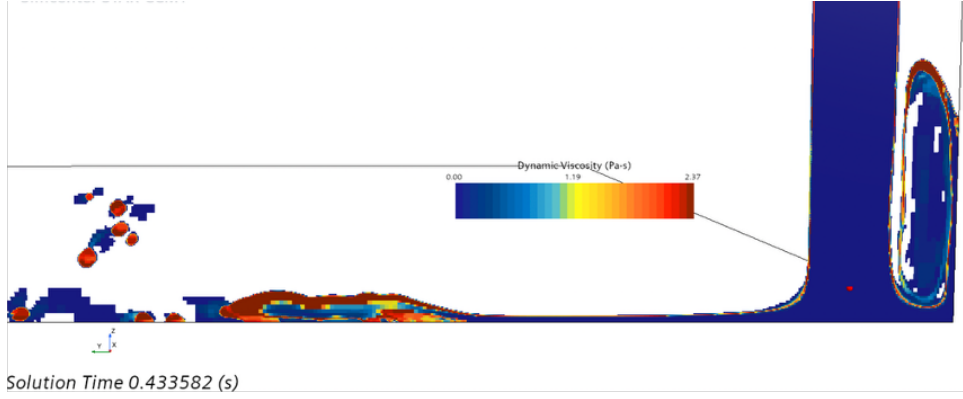


Figure 4.16: Dynamic viscosity contour for Case 3B.

This behaviour confirms that the Ramacciotti coefficient has a direct impact on the predicted spreading. A lower value of (C) allows the melt to remain mobile for longer, but it does not provide enough resistance to reproduce the accumulation observed experimentally.

4.5.4. Effect of the Ramacciotti coefficient on melt mobility

The comparison between Cases 3A and 3B shows that the Ramacciotti coefficient controls the balance between spreading and immobilisation. With $C = 2$ the viscosity increase is too weak to form a stable accumulation at the impact point, so that the melt keeps spreading as a thin mobile layer; with $C = 4$ the model produces a stronger reduction of mobility and a more evident accumulation of material after impact. This refers to the ability to build up a localised deposit, rather than to the front propagation itself, which remains broadly comparable to the experiment in both cases.

The melt-front plots in the X - and Y -directions (Figures 4.18a and 4.18b) confirm this trend. The cases with Ramacciotti viscosity predict a slower front progression than the experimental reference, especially when $C = 4$. This does not necessarily mean that $C = 4$ is globally less suitable: from the point of view of the impact-region behaviour, $C = 4$ better reproduces the tendency of the melt to accumulate and lose mobility. The spatial distribution, however, is still not fully consistent with the experiment, because the material does not build up in the impact zone in the same way as observed in PULiMS-E10.

To clarify the reference system adopted for the melt spreading analysis, Figure 4.17 shows the inlet nozzle position and the spatial directions used in the post-processing. The red circle identifies the melt inlet nozzle, while the x -, y -, and z -directions indicate the

reference directions considered for the evaluation of melt spreading.

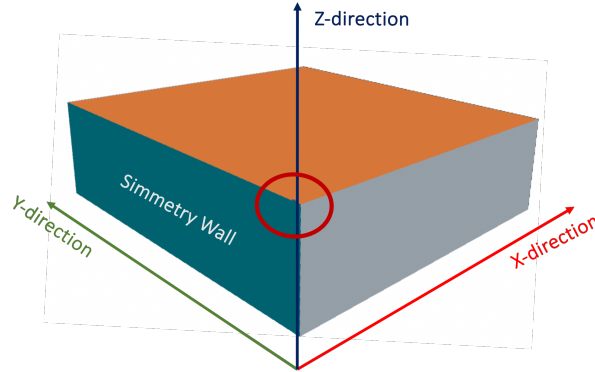
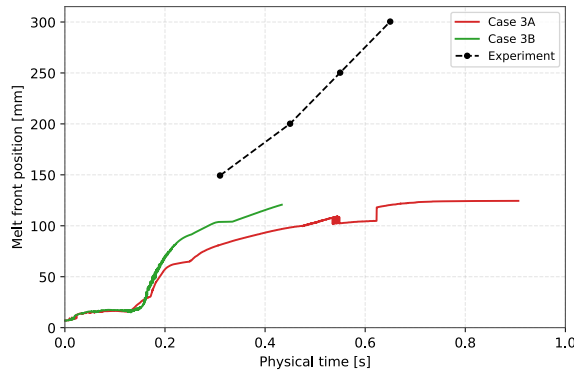
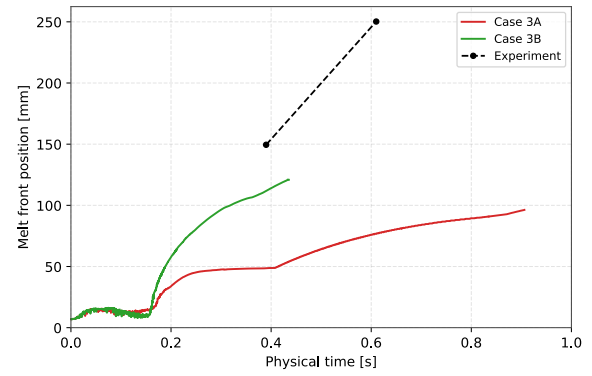


Figure 4.17: Reference system adopted for the melt spreading analysis for all the cases.



(a) X-direction.



(b) Y-direction.

Figure 4.18: Case 3: melt front position in the X - and Y -directions for $C = 4$ (Case 3A) and $C = 2$ (Case 3B), compared with the experimental reconstruction. Experimental data from [14].

The reconstructed melt temperature at the central impact-zone thermocouple is reported in Figure 4.19. In both Cases 3A and 3B the melt reaches the centre of the plate at $t \approx 0.15$ s, in agreement with the onset of the experimental signal; afterwards the reconstructed temperature stays close to the melt value, indicating that, with the activation depth used in Case 3, the melt continuously fed into the impact region is not strongly cooled. This is consistent with the limited and displaced accumulation observed at the impact point and with the inability of these cases, by themselves, to immobilise the melt where it first reaches the plate.

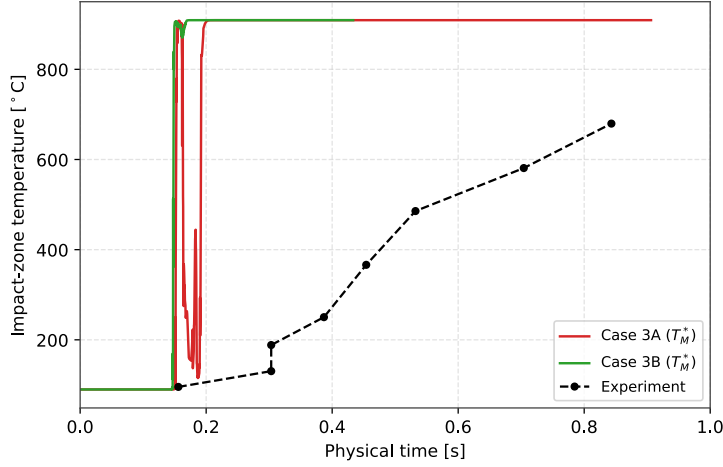


Figure 4.19: Case 3: reconstructed melt temperature T_M^* at the impact-zone thermocouple for $C = 4$ (Case 3A) and $C = 2$ (Case 3B), compared with the experimental TC0. Experimental data from [14].

4.5.5. Limitations of Case 3

Although the Ramacciotti model improves the representation of melt immobilisation compared with the constant-viscosity case, Cases 3A and 3B still do not reproduce the experimental impact behaviour satisfactorily. In the experiment, the first material reaching the pool bottom forms a deposit in the impact region, while the following hotter melt continues to spread over it. In the simulations, instead, the local accumulation appears displaced from the impact zone, with a depression close to the jet impact location and a higher ridge around it.

This result indicates that the viscosity model alone is not sufficient. The onset and intensity of the heat extraction in the impact region must also be modified. Case 4 therefore introduces an enhanced volumetric heat extraction – obtained by multiplying the volumetric heat flux by a factor A inside a confined impact-region control volume – together with a deeper activation level.

4.6. Case 4: Modified heat-transfer activation and enhanced volumetric heat extraction

Case 4 was introduced to improve the behaviour observed in Case 3. Although the Rameciotti viscosity model reduced the melt mobility, the accumulation pattern was still not satisfactory in the impact region. For this reason, the thermal treatment was modified by increasing the activation depth from 0.1212 m to 0.16 m and by introducing an enhanced volumetric heat extraction inside a prescribed impact region.

It is worth clarifying why the activation depth was increased rather than decreased. Since z_{act} is measured from the free surface, a larger value moves the onset of the melt–water heat exchange closer to the bottom plate (from 0.0788 m to 0.04 m above the floor). Increasing z_{act} therefore keeps the melt thermally insulated for almost the entire descent – consistently with the film-boiling picture described in Section 2.5 – and concentrates the cooling, and the consequent loss of mobility, in the impact region, where the experiment shows the first accumulation. Decreasing z_{act} would have the opposite effect: it would activate the heat exchange higher in the pool, cooling the melt prematurely during the fall and immobilising it before it reaches the plate, in contrast with the observed behaviour.

The impact region was defined as a cubical control volume centred around the expected impact area of the melt. Its horizontal dimensions are 0.04 m by 0.04 m, while its vertical extension is equal to $H = 0.2 - 0.16 = 0.04$ m. Inside this region, the volumetric heat flux is multiplied by a factor $A = 1000$. This modification is not intended to represent a directly measured local heat-transfer coefficient, but rather to force a stronger local cooling in the region where the first melt accumulation is experimentally expected. The selected impact-region control volume is shown, from different viewpoints, in Figure 4.20.

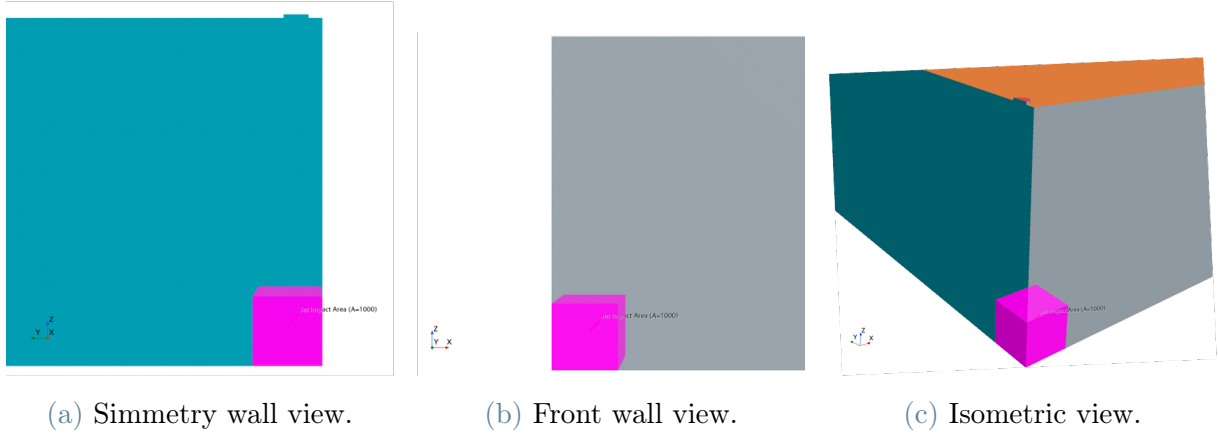


Figure 4.20: Views of the cubic control volume in which the thermal exchange term is activated, with $A = 1000$ multiplying the volumetric heat flux.

Two cases were analysed. Case 4A uses $C = 4$ and was simulated up to approximately $t = 0.51$ s. Case 4B uses $C = 2$ and was simulated up to approximately $t = 0.24$ s. The comparison between the two cases allows the effect of the enhanced heat extraction to be separated from the effect of the viscosity-growth coefficient.

4.6.1. Case 4A: Activation depth equal to 0.16 m, $C = 4$ and $A = 1000$

In Case 4A, the combination of enhanced heat extraction and $C = 4$ produces a clear local immobilisation of the melt in the impact region. Compared with Case 3A, the material is arrested closer to the initial impact area, and a more evident deposit is formed below the incoming jet. The temperature, viscosity and velocity contours on the symmetry wall are reported in Figure 4.21.

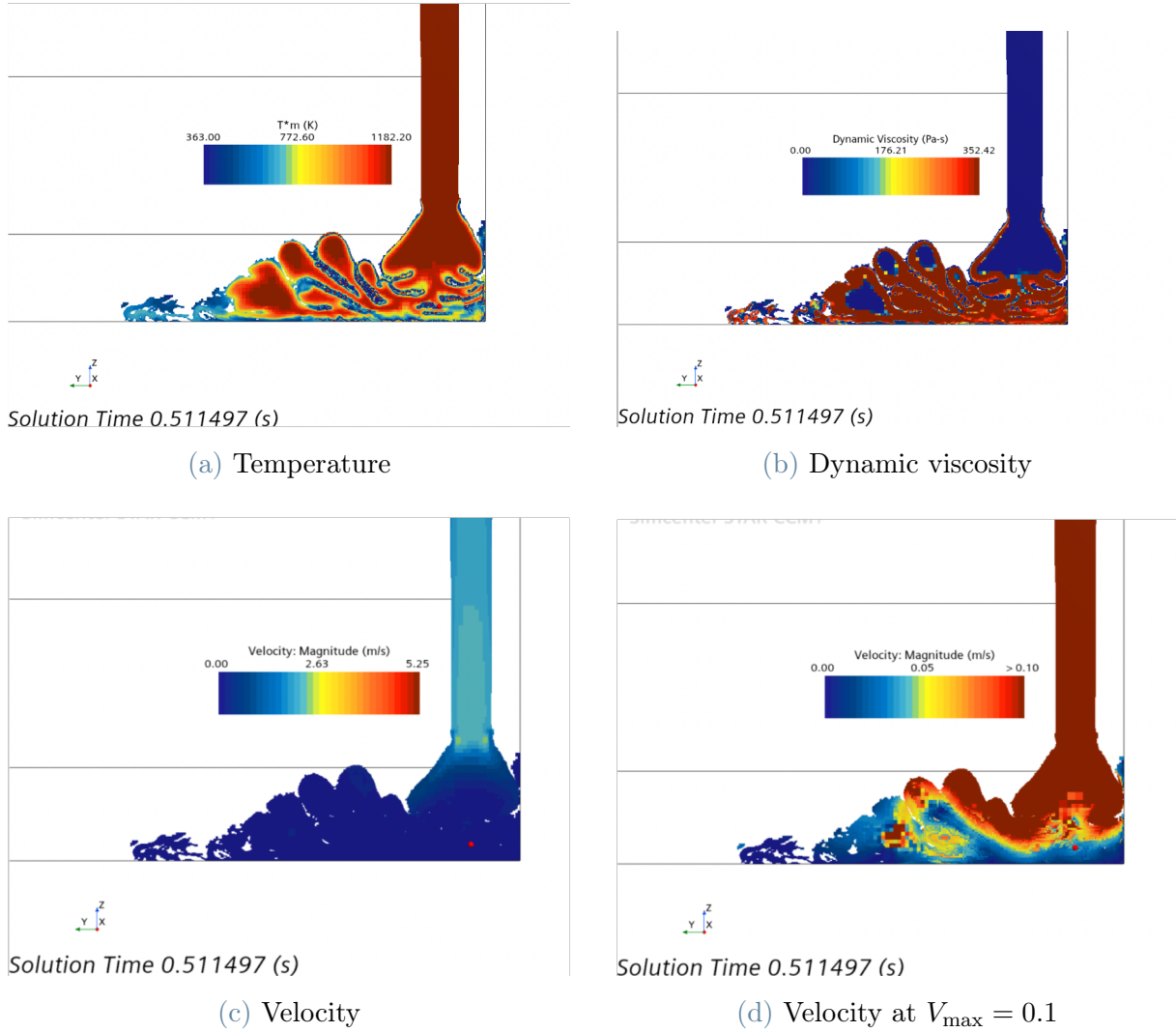


Figure 4.21: Symmetry-wall contours for Case 4A.

The velocity field confirms that the enhanced cooling region strongly reduces the mobility of the melt near the pool bottom. The material in contact with the impact region slows down and accumulates, while the incoming jet remains continuous. This is an important improvement with respect to Case 3, where the main accumulation was displaced from the impact location.

This local immobilisation, however, comes together with a limitation that is intrinsic to the modelling approach. Since the melt is represented through a VOF formulation as a continuous phase, the incoming material remains a coherent structure rather than breaking up: the jet stays connected to the deposited layer, and the fragmented or granular spreading suggested by the experimental observations cannot be reproduced. This is consistent with the behaviour found here: while the local deposit at the impact point is

improved with respect to Case 3, the lateral expansion of the melt in the pool remains more limited than in the experiment.

4.6.2. Case 4B: Activation depth equal to 0.16 m, $C = 2$ and $A = 1000$

Case 4B uses the same activation depth and the same heat-extraction multiplier as Case 4A, but with a lower Ramacciotti coefficient ($C = 2$). The resulting viscosity increase is weaker, and the melt remains more mobile after entering the impact region, as shown by the symmetry-wall contours in Figure 4.22.

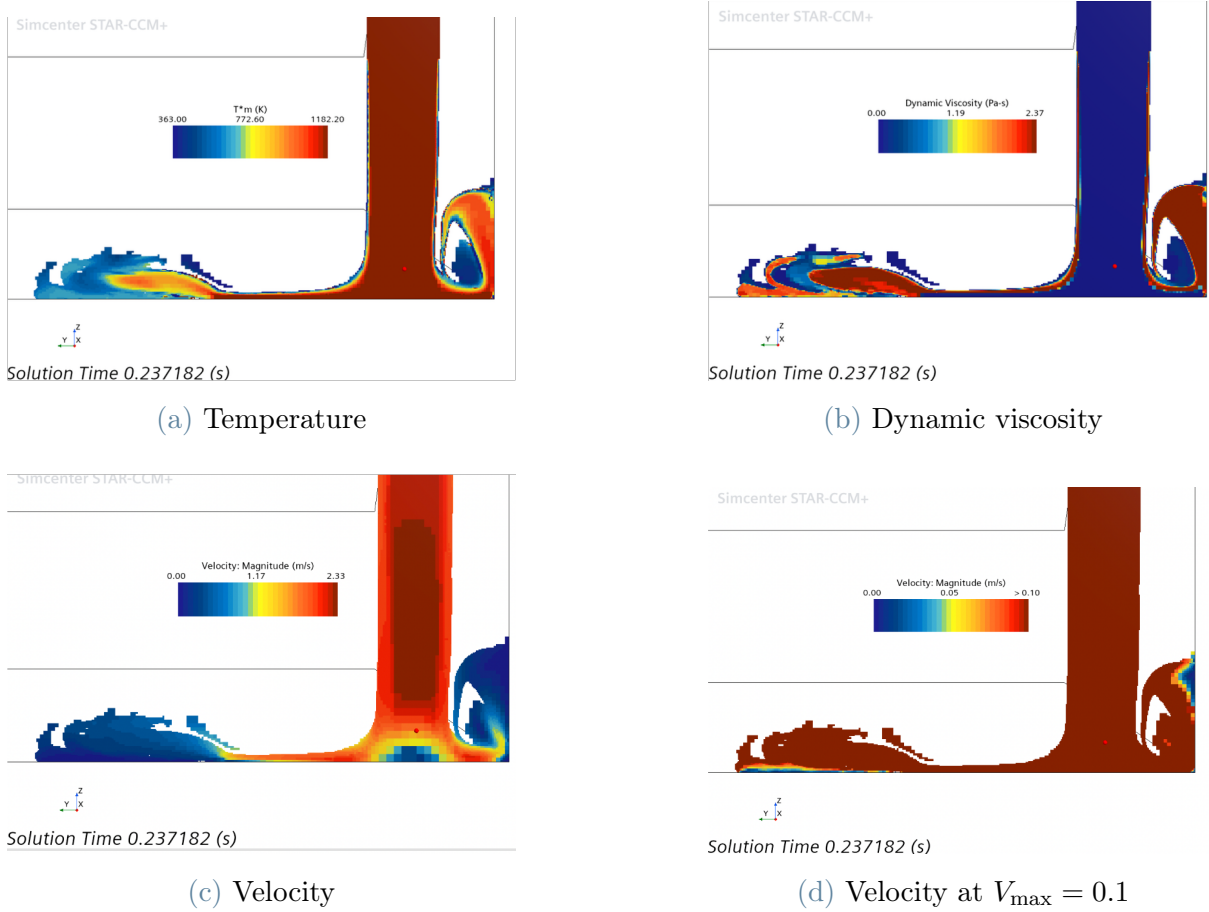


Figure 4.22: Symmetry-wall contours for Case 4B.

The lower value of C reduces the effect of the enhanced cooling region. Although the thermal source term is intensified by the same factor $A=1000$, the viscosity response is not strong enough to produce a stable accumulation comparable to Case 4A. The melt remains too mobile and continues to spread without forming a sufficiently localised deposit in the impact zone.

This confirms that the enhanced heat extraction alone is not sufficient. A sufficiently strong coupling between solid fraction and viscosity is also required. In this respect, Case 4A provides a more representative behaviour than Case 4B.

4.6.3. Effect of the enhanced heat-extraction region

The comparison with Case 3 indicates that the impact-region source term changes the local behaviour of the melt. In Case 3, the viscosity increase was governed only by the phase-temperature state and by the Ramacciotti law. The resulting accumulation occurred mainly after the initial impact region, producing a depression below the jet and a ridge around it. In Case 4A, instead, the additional heat extraction promotes immobilisation directly in the impact region.

This modification therefore improves the qualitative agreement with the expected experimental behaviour, where the first material reaching the pool bottom rapidly loses mobility and forms a deposit over which hotter melt can subsequently flow [14]. Nevertheless, the simulation does not fully reproduce this mechanism. The melt still behaves as a continuous VOF structure, and the spreading over the already deposited material remains limited.

4.6.4. Effect on melt accumulation and spreading

The melt-front comparison in the X - and Y -directions (Figures 4.23a and 4.23b) confirms that the enhanced heat extraction reduces the spreading with respect to the experimental reference. In particular, Case 4A shows a stronger arrest of the melt front, while Case 4B allows a larger motion because of the lower viscosity-growth coefficient.

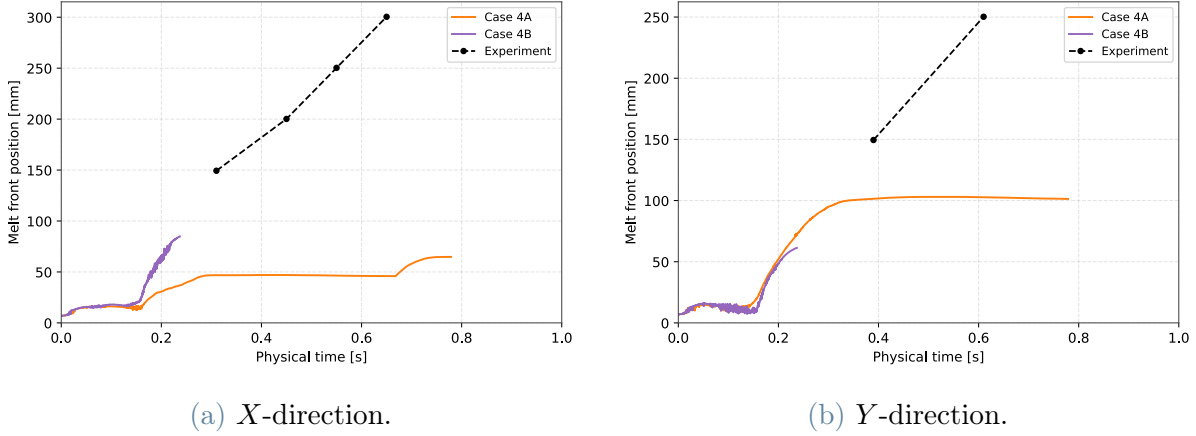


Figure 4.23: Case 4: melt front position in the X - and Y -directions for $C = 4$ (Case 4A) and $C = 2$ (Case 4B), compared with the experimental reconstruction. Experimental data from [14].

The clearest signature of the enhanced impact-region extraction is found in the impact-zone temperature, reported in Figure 4.24. As in the other cases, the melt reaches the centre of the plate at $t \approx 0.15$ s. In Case 4A, however, the reconstructed temperature T_M^* is subsequently driven repeatedly and sharply below the melt value, down to a few hundred degrees Celsius: this is the strong, localised cooling produced by the impact-region heat sink, which through the Ramacciotti law immobilises the melt at the impact point. In Case 4B the weaker viscosity response keeps the melt mobile and T_M^* closer to the melt temperature. The experimental thermocouple, by contrast, heats gradually over several seconds towards about 890°C , reflecting the persistent hot melt accumulated on the sensor; the pronounced cooling of T_M^* in Case 4A must therefore be read as a deliberate modelling device to trigger local immobilisation, rather than as the absolute temperature of the deposit.

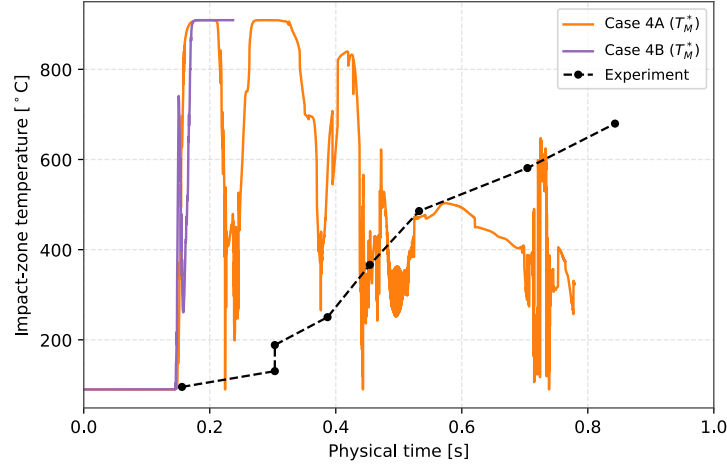


Figure 4.24: Case 4: reconstructed melt temperature T_M^* at the impact-zone thermocouple for $C = 4$ (Case 4A) and $C = 2$ (Case 4B), compared with the experimental TC0. Experimental data from [14].

Overall, Case 4A represents an improvement in terms of local deposition, because the melt starts to accumulate closer to the impact area. At the same time, the predicted lateral spreading is still too limited. This suggests that the missing mechanism is not only thermal immobilisation, but also the hydrodynamic effect of the vapour layer observed during melt-water interaction.

4.7. Summary of the sensitivity analysis

The numerical campaign presented in this chapter explored the effect of three main modelling parameters on the predicted melt spreading behaviour: the Ramacciotti viscosity coefficient C , the heat-exchange source-term activation depth z_{act} , and the volumetric heat-flux multiplier A applied within the impact-region control volume introduced in Case 4. Table 4.3 collects the parameter combinations investigated across all cases, together with the corresponding qualitative outcome in terms of melt mobility and impact-region accumulation.

Table 4.3: Summary of the parameters varied in the sensitivity analysis and their qualitative effect on the predicted spreading behaviour.

Case	C	z_{act} [m]	Impact region	A	Qualitative outcome
1	–	–	No	–	Direct energy-equation solution; unphysical melt cooling observed during fall even with negligible thermal conductivity. Motivated the two-temperature approach.
2	–	0.1212	No	–	Two-temperature thermal model validated; melt temperature correctly preserved during fall. Constant viscosity (0.016 Pas); melt remains too mobile, no accumulation.
3A	4	0.1212	No	–	Ramacciotti coupling active; viscosity increase reduces spreading but accumulation is displaced from the impact point (depression at impact, ridge around it).
3B	2	0.1212	No	–	Weaker viscosity growth; melt remains highly mobile, no stable accumulation forms.
4A	4	0.16	Yes (0.04 m cube)	1000	Enhanced local heat extraction produces clear local immobilisation near the impact point; best qualitative agreement with expected impact-region behaviour among the cases analysed.
4B	2	0.16	Yes (0.04 m cube)	1000	Enhanced heat extraction alone is insufficient without a sufficiently strong C ; melt remains too mobile despite the same thermal source term as 4A.

Three trends can be identified from this comparison.

Effect of the Ramacciotti coefficient C . Across all activation-depth and impact-region configurations, increasing C from 2 to 4 consistently produced a stronger reduction in melt mobility and a more localised accumulation (compare Cases 3A vs. 3B, and 4A vs. 4B). The higher reference value $C = 6.1$, reported in the original Ramacciotti formulation for the specific corium-representative material considered in [21], was tested in a preliminary run and discarded, since it produced a near-complete and physically unrealistic immobilisation of the jet within the present framework.

Effect of the activation depth z_{act} . Increasing z_{act} from 0.1212 m to 0.16 m, combined with the introduction of the impact-region heat source, shifted the onset of significant cooling closer to the floor, consistent with the physical picture of a thermally insulated falling stage followed by a thermally active spreading stage (Section 2.5).

Effect of the impact-region heat-flux multiplier A . The comparison between Cases 3 and 4 indicates that the activation depth and the Ramacciotti coefficient alone are not sufficient to reproduce a localised accumulation at the impact point: only the introduction of the spatially confined, strongly enhanced heat sink in Case 4 produced an accumulation pattern consistent with the interpretation discussed in Section 2.5.2. The value $A = 1000$ adopted in Case 4 was not derived from a resolved heat-transfer coefficient, but was selected as the order of magnitude required to produce a visible local immobilisation effect within the simulated time window.

Melt front propagation velocity. The melt front velocity in the Y -direction ($+90^\circ$), obtained by differentiating the front position, is compared with the experimental estimate (reconstructed from the 2000 fps video recordings) in Figure 4.25. The numerical cases reproduce an intense but very short initial spreading burst: the front velocity peaks around $t \approx 0.18$ s, when the jet first impacts and spreads on the plate, and then decreases rapidly. The experimental front, instead, reaches a comparable peak (about 780 mm/s) slightly later, around $t \approx 0.35$ s, and sustains a high velocity (roughly 400–540 mm/s) up to about 0.7 s. The numerical fronts therefore decelerate and arrest much earlier than the experimental one, most markedly in Case 4A, where the enhanced impact-region extraction brings the front velocity close to zero within a few tenths of a second. This confirms, now also in terms of velocity, that the model captures the early spreading impulse but underestimates the persistence of the lateral propagation observed experimentally.

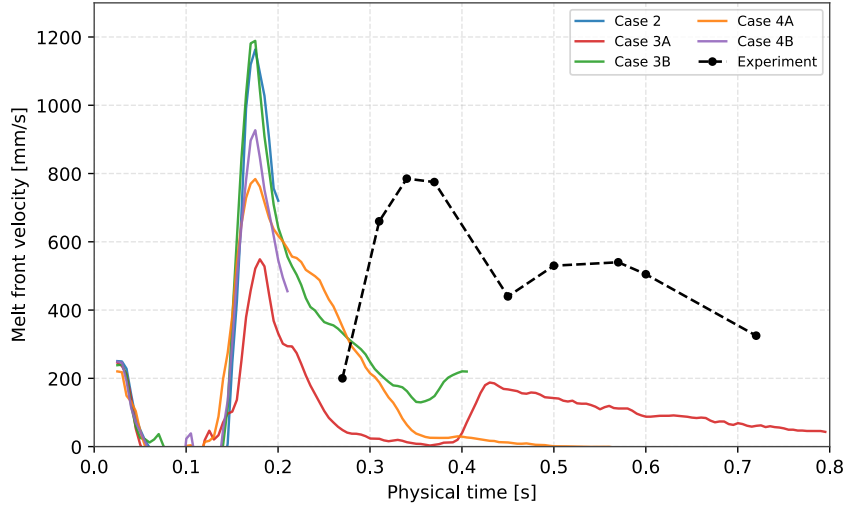


Figure 4.25: Melt front propagation velocity in the Y -direction ($+90^\circ$): numerical cases, obtained by differentiating the front position, compared with the experimental estimate from the 2000 fps video recordings [14].

Overall, the sensitivity analysis indicates that the final spreading and accumulation pattern predicted by the present model is controlled by the combined effect of these three parameters rather than by any single one in isolation: the Ramacciotti coefficient C governs the intensity of the rheological response once cooling occurs, the activation depth z_{act} governs when cooling is allowed to begin, and the impact-region multiplier A governs where cooling is locally enhanced. None of these parameters was calibrated through a formal optimisation procedure; their values were instead selected through a sequential, physically motivated exploration, as documented throughout this chapter. This is an inherent limitation of the present modelling strategy, discussed further in Chapter 5.

5 | Conclusions

5.1. Summary and main findings

This thesis investigated the underwater spreading of a high-temperature melt in the PULiMS-E10 experiment by means of a transient, three-dimensional Volume of Fluid simulation developed in Simcenter STAR-CCM+. The objective was not to resolve every microscopic phenomenon of the melt–coolant interaction, but to build a computationally affordable model able to reproduce the dominant features of the spreading process and, in particular, to capture the influence of the cooling-induced rheological evolution of the melt on its final distribution over the bottom plate.

The central modelling choice of the work was to describe the thermal field with two separate transport equations for the phase temperatures, one for the melt and one for the water, rather than with a single mixture energy equation, while neglecting the vapour phase. This decision was motivated by a specific, reproducible artefact: a single mixture energy equation produced a spurious cooling of the melt during the falling stage even when the thermal conductivity was set to a near-zero value. The two-dimensional test case discussed in Chapter 4 isolated the origin of this behaviour, showing that the apparent cooling is not a resolved conductive process but a numerical interface-transport error, produced by the averaging of the two very different phase temperatures within the interfacial cells and amplified by a coarse temporal resolution. The same test confirmed that transporting the two phase temperatures separately preserves the bulk melt temperature and confines the thermal exchange to the interfacial cells, thus justifying the strategy adopted for the full simulations.

On this basis, the melt–water heat exchange was activated only below a prescribed depth, to mimic, in a simplified and binary way, the insulating effect of film boiling around the falling jet, and the reconstructed melt temperature was used to evaluate an equivalent solid fraction feeding the Ramacciotti viscosity law. The numerical campaign was organised as a sequence of cases of increasing complexity, which made it possible to clarify the role of each modelling ingredient: Case 1 demonstrated the inadequacy of the single mixture

temperature equation; Case 2 validated the two-temperature thermal model with constant viscosity; Cases 3A and 3B introduced the Ramacciotti coupling and quantified the effect of the viscosity-growth coefficient C ; and Cases 4A and 4B added an enhanced, spatially confined heat extraction in the impact region. The reference value $C = 4$, retained for the present analysis, was found to provide the best compromise between mobility and immobilisation, in agreement with the value independently adopted in the literature for a comparable problem [28].

A specific physical contribution of this work concerns the interpretation of the impact region. Whereas the molten jet quench model and the original PULiMS reports attribute the diffuse, light-coloured region observed around the impingement point to vapour driving the fragmentation of the jet, a closer inspection of the high-speed recordings supports a different reading: the cloud is interpreted as melt that has already undergone rapid surface solidification and local accumulation upon contact with the subcooled water and the plate. This reinterpretation is the physical motivation for the enhanced heat-extraction region introduced in Case 4, which reproduces a localised, thermally driven immobilisation of the melt at the impact point rather than a vapour-driven fragmentation.

When compared with the experimental measurements, the model proved able to reproduce correctly the time at which the melt jet reaches the centre of the spreading plate, with the impact-zone temperature rising at $t \approx 0.15$ s in all cases, consistently with the onset of the experimental thermocouple signal. The enhanced extraction of Case 4A produced the intended strong local cooling of the reconstructed temperature and the consequent immobilisation of the melt close to the impingement point, in qualitative agreement with the experimental evidence of an early, persistent deposit. At the same time, the comparison of the melt front position and velocity showed that the model captures the initial spreading impulse but systematically underestimates both the extent and the persistence of the lateral propagation: the numerical fronts decelerate and arrest much earlier than the experimental one. Overall, the model provides a consistent and physically interpretable description of the dominant spreading dynamics and of the role of cooling-induced viscosity increase, while not reproducing the full lateral extent of the experimental spread.

5.2. Limitations and future developments

The results must be read in the light of the simplifying assumptions on which the model is built. The thermal field is described by two phase-temperature transport equations and the melt–water heat exchange by a simplified, depth-activated source term; the vapour phase is not modelled, so that film boiling is reproduced only through its insulating

effect during the fall, without resolving the vapour film or its collapse. Solidification is introduced through the viscosity law rather than through a resolved enthalpy balance; melt fragmentation and the internal porous, multi-layer morphology of the final debris bed are not represented, although the model does reproduce the formation of a coherent solid accumulation of melt at the impact region. The simulated physical time is, moreover, limited to a fraction of a second, shorter than the experimental spreading time, so that the quantitative comparison concerns mainly the early stages of the process.

Several developments can be envisaged to build on the present work, while remaining consistent with the modelling framework adopted here. The first is the introduction of an effective reduction of the hydrodynamic resistance experienced by the melt during the melt–water interaction — for instance through a reduced effective density of the surrounding phase in the momentum balance — in order to recover the larger lateral spreading observed experimentally. The second is the extension of the simulated physical time, which would allow a more complete comparison with the later stages of the experimental spreading and a fuller assessment of the final melt distribution. A further refinement would be a more systematic calibration of the empirical parameters of the model — the Ramacciotti coefficient, the activation depth and the impact-region heat-flux multiplier — against the available experimental data, so as to place their selection on a firmer quantitative basis.

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A | Appendix A

Appendix A

User-defined field functions

This appendix reports the main user-defined field functions implemented in STAR-CCM+ for the numerical simulations discussed in Chapter 4. The functions are reported using the original STAR-CCM+ syntax adopted in the model.

Reference enthalpy scale

The field function H_0 defines the reference volumetric enthalpy scale used to reconstruct the melt and water temperature fields from the two transported scalars.

H_0 :

$$\rho_{\text{Bi203-W03}} \cdot 280 \cdot (909.2 - 90)$$

Reconstructed temperature fields

The reconstructed melt temperature, T^*_m , is obtained from the transported scalar associated with the melt phase. The upper bound is imposed to keep the reconstructed temperature below the initial melt temperature.

T^*_m :

$$\min(363 + H_0 \cdot \Phi_{\text{Melt}} / (\rho_{\text{Bi203-W03}} \cdot 280), 1182.2)$$

The reconstructed water temperature, T^*_w , is obtained from the transported scalar associated with the water phase. The lower bound is imposed to avoid values below the initial water temperature.

T^*_w :

```
max(363+${H0}*${Phi_Water}/(965*4205), 363)
```

Thermal source terms

The source terms for the melt and water transported scalars are activated only below the prescribed activation depth. The expressions below refer to the case with activation depth equal to 0.16 m. For the cases with activation depth equal to 0.1212 m, the same formulation was used by replacing -0.16 with -0.1212.

Source_Melt:

```
($$Position[2] < -H) ? (-${q''_th}/${H0}) : 0
```

Source_Water:

```
($$Position[2] < -H) ? (${q''_th}/${H0}) : 0
```

Interfacial heat-transfer term

The field function q''_{th} defines the heat-transfer term between melt and water. In the cases including the impact-region correction, the term is multiplied by a factor equal to 1000 inside the selected region.

q''_{th} :

```
(($$Position[0] > -H) && ($$Position[1] < H)) ?  
1000*(((${T*m}-${T*w})*${mag(grad(alpha_m))})/  
(${delta(n)}*(1/5.3+1/0.62))) :  
(((${T*m}-${T*w})*${mag(grad(alpha_m))})/  
(${delta(n)}*(1/5.3+1/0.62)))
```

Interface-related auxiliary functions

The function $\delta(n)$ estimates the local characteristic cell length from the cell volume.

$\delta(n)$:

```
pow(${Volume}, 1/3)
```

The function $\text{mag}(\text{grad}(\alpha_m))$ evaluates the magnitude of the melt volume-fraction gradient and is used to localise the interfacial heat-transfer contribution.

```
mag(grad(alpha_m)):
mag(grad(${VolumeFractionBi203-W03}))
```

Auxiliary normalised temperature

The auxiliary variable T_{star} is defined as a normalised melt temperature. It is used to reconstruct the solid volume fraction by mapping the reconstructed melt temperature between the selected liquidus and solidus reference temperatures.

```
T_star:
(${T*m}-1143)/(1189-1143)
```

Solid volume fraction reconstruction

The solid volume fraction is reconstructed from the auxiliary variable T_{star} . The value is limited between 0 and 1.

```
Solid_Volume_Fraction*:
(${T_star} > 1) ? 0 : (${T_star} < 0) ? 1 : (1-${T_star})
```

For visualisation purposes, the same quantity was also filtered using the melt volume fraction, so that the solid fraction is displayed only where the melt phase is present.

```
Animation_Solid_Volume_Fraction*:
(${VolumeFractionBi203-W03}>0.01) ?
(((${T_star} > 1) ? 0 : (${T_star} < 0) ? 1 : (1-${T_star}))) : 0
```

Ramacciotti viscosity model

The Ramacciotti viscosity model was implemented as a user-defined field function depending on the reconstructed solid volume fraction. The expression below refers to the case with coefficient C equal to 4. For the simulations with C equal to 2, the coefficient 4 was replaced by 2.

```
Ramacciotti:
0.016 * exp(2.5*C*${Solid_Volume_Fraction*})
```

Melt density functions

The melt density was defined as a function of the reconstructed melt temperature. A constant value was imposed below the selected temperature threshold.

Melt_Density:

$$(\{T_m\} > 1143) ? (-1.172 * (\{T_m\} - 273) + 7896) : 7838$$

The corresponding derivative with respect to temperature was introduced as an auxiliary field function.

Melt_Density_Temperature_Derivative:

$$(\{T_m\} > 1143) ? -1.1172 : 0$$

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List of Symbols

Symbol	Description	Unit
<i>Latin symbols</i>		
A	impact-region heat-flux multiplier	–
c_p	specific heat capacity	J/(kg K)
C	Ramacciotti viscosity coefficient	–
f_s	equivalent solid volume fraction	–
$\mathbf{g}$	gravitational acceleration	m/s ²
h	specific enthalpy	J/kg
H_0	reference volumetric sensible enthalpy	J/m ³
k	thermal conductivity	W/(m K)
$\dot{m}$	melt mass flow rate	kg/s
$\mathbf{n}$	outward unit normal vector	–
p	pressure	Pa
$\dot{q}_{th}''$	interfacial heat flux	W/m ²
$\dot{q}_{th}'''$	volumetric heat-transfer rate	W/m ³
r	nozzle radius	m
R_{eq}''	equivalent interfacial thermal resistance	m ² K/W
S	source term (generic)	–
t	time	s
T	temperature	K
T_M^*, T_W^*	reconstructed melt and water temperature	K
$T_{M,in}$	melt inlet temperature	K
T_{ref}	reference temperature	K
T_{sol}, T_{liq}	solidus and liquidus temperature	K
T^*	normalised melt temperature	–
$\mathbf{u}$	velocity vector	m/s
v_0	melt velocity at the nozzle outlet	m/s
v_{in}	melt velocity imposed at the inlet	m/s

Symbol	Description	Unit
V	cell volume	m^3
z_{act}	source-term activation depth	m
<i>Greek symbols</i>		
α_i	volume fraction of phase i	—
Δn	characteristic interfacial cell length	m
Δt	time step	s
μ	dynamic viscosity	Pa s
μ_0	dynamic viscosity of the fully liquid melt	Pa s
ρ	density	kg/m^3
σ	melt–water surface tension	N/m
ϕ_M, ϕ_W	melt and water transported scalar	—
<i>Subscripts</i>		
M	melt phase	
W	water phase	
m	mixture	
eff	effective	
<i>Acronyms</i>		
AMR	Adaptive Mesh Refinement	
CFD	Computational Fluid Dynamics	
CFL	Courant–Friedrichs–Lewy (number)	
DEFOR	Debris Bed Formation	
FCI	Fuel–Coolant Interaction	
IEA	International Energy Agency	
KTH	Royal Institute of Technology (Sweden)	
LWR	Light Water Reactor	
MCCI	Molten Core–Concrete Interaction	
NRA	Nuclear Regulation Authority (Japan)	
PULiMS	Pouring and Underwater Liquid Melt Spreading	
REMCOD	Remelting of Multi-Component Debris	
RPV	Reactor Pressure Vessel	
TC	Thermocouple	
VOF	Volume of Fluid	

